Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

May 10, 2017

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HECC Teams Crunch PLC Data from Modular Supercomputer Facility

- The HECC Tools and Facilities teams collaborated to develop a set of operational charts, based on data derived from the Modular Supercomputing Facility (MSF) Programmable Logic Controller (PLC), which present key MSF performance characteristics.
- The PLC outputs 1,300 data points every 10 seconds from the MSF's instrumentation. When more than 11 million data points per day proved too much to maintain within an Excel spreadsheet, the Tools team developed a Python script to parse the data and created custom graphs to evaluate MSF performance.
  - The graphs provide operating trends over user-selected time periods.
  - Metrics such as Power Utilization Effectiveness (PUE), power consumption, the temperature change (ΔT) from the front to back of the racks, cold aisle temperature/ outside temperature/water used, and damper orientation are trended.
- Anticipating the performance trends of the MSF helps identify the operating health of the system to assist with maintenance, allows for operating changes to be measured, and identifies areas that need improvement.

Mission Impact: The ability to trend performance data to drive improvements and identify system operational health improves the Modular Supercomputing Facility's uptime availability and power/cooling efficiency.

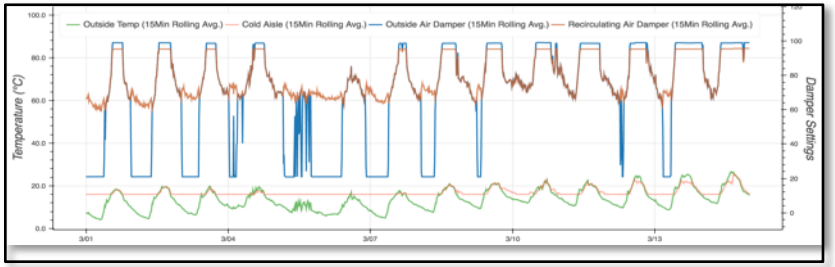


Chart showing the position of the outside air dampers and recirculating air dampers in relation to the outside air and cold aisle temperatures for the MSF. As the outside air temperature (green) drops, the outside air dampers (blue) close, and the recirculating air dampers (orange) open to maintain a cold aisle temperature of 16-20 degrees Celsius.

POCs: Chris Tanner, christopher.tanner@nasa.gov, (650) 604-6754, Vidya Bobbiligama, vidyareddy.bobbiligama@nasa.gov, (650) 604-4460, NASA Advanced Supercomputing Division, CSRA LLC

Facilities Team Tests Evaporative Cooling in Modular Supercomputer Facility

- The HECC Facilities team took advantage of unseasonably warm weather in late March to test the evaporative cooling system in the Modular Supercomputer Facility (MSF). They lowered the set point temperature for the cold aisle to force the module to use its adiabatic system for cooling.
- The evaporative cooling system and controls worked flawlessly and kept the cold aisle below its maximum temperature set point.
  - The cold aisle temperature tracked the outside temperature until the 23.9°C cold aisle set point was reached and the MSF control system flowed water over the evaporative media, cooling the air down to 21°C before it entered the cold aisle.
  - The evaporative system achieved the temperature adjustment with only 1/3 of the maximum water flow.
  - This sensitive control system even detected when the outside air dropped below the set point, and stopped the flow of water.
- The cooling system test provides the Facilities team with confidence that the MSF will be capable of delivering properly conditioned air to the computer system throughout the year. The cold aisle set point for production operation is 27°C—the higher the cold aisle set point, the less water used within the MSF.

Mission Impact: The ability to run the MSF year-round without direct expansion cooling means that money saved on power can be used to provide more compute resources to HECC users. The evaporative cooling system also uses less than 1% of the water used by direct expansion cooling.

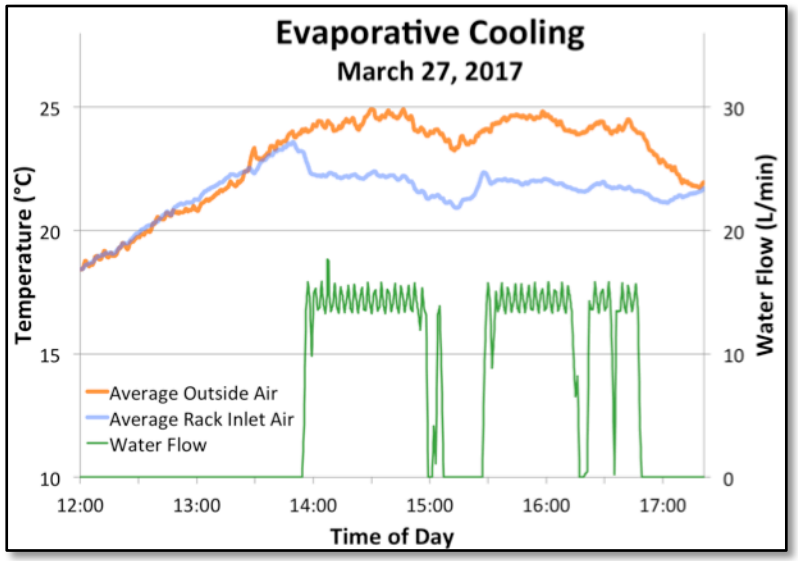


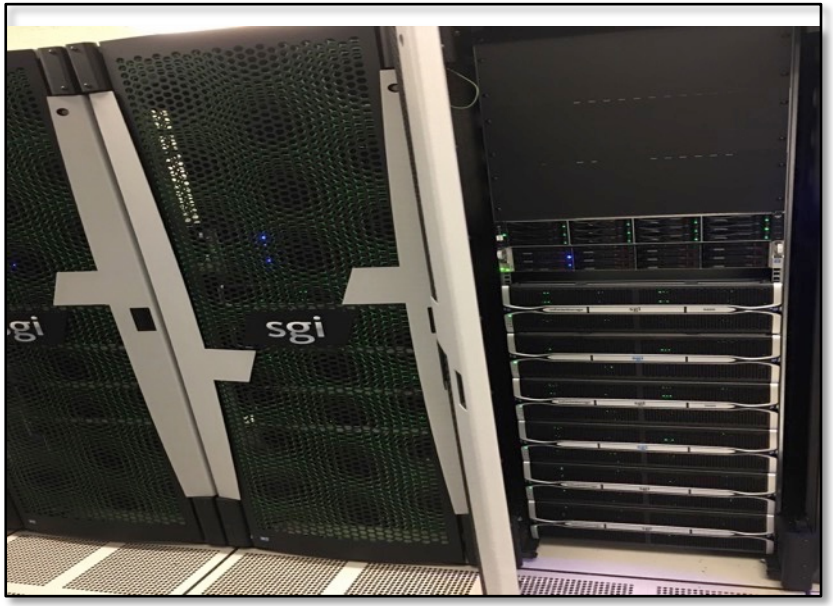
Chart showing the impact of MSF evaporative cooling on the rack inlet air temperature (blue). While the outside temperature continued to climb (orange), the water flow to evaporative media (green) has the effect of lowering temperature by 3 degrees Celsius. During the 5-hour test, ~500 gallons of water were used.

POCs: Chris Tanner, christopher.tanner@nasa.gov, (650) 604-6754, NASA Advanced Supercomputing Division, CSRA LLC

HECC Collaborates with Vendor to Improve Lustre Filesystem Performance

- HECC engineers improved the performance of the visualization filesystem, nobackupp1, augmenting the capacity by 2.8 petabytes (PB) to provide the storage required for large-scale visualizations.
- After the capacity increase, visualization and systems staff noticed inconsistent performance on the filesystem, and that the new storage was slower than the original storage.
- HECC engineers worked with Hewlett Packard Enterprise to develop a method that improved performance without requiring the remaking of the filesystem, which would have been highly disruptive and time consuming.
- After implementing the change, performance improved from 5.2 GB/s to 5.5 GB/s, with the largest improvement on the new disks, from 4.2 GB/s to 5.5 GB/s. There was a slight decrease on the original storage performance, from 5.7 GB/s to 5.5 GB/s, but overall performance and consistency improved.

Mission Impact: Optimizing the performance of HECC resources enables users to more fully utilize the computing resources and run more data-intensive applications for NASA research projects.



By relocating the disk drives within the RAID subsystem, HECC and Hewlett Packard Enterprise engineers made the Lustre filesystem's performance more consistent. This method will also be utilized when the noackupp2 filesystem is expanded.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division;
Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, CSRA LLC

APP Experts Help Projects Make the Best Use of Their Allocations

- Over the last three months, experts in the HECC Application Performance and Productivity (APP) team handled over 200 Remedy tickets from users. A sampling of the help they provided includes:
  - An ARMD project from Langley experienced data corruption when users tried building their application with the latest Intel compiler. The APP team isolated the issue as a bug in the compiler's runtime library, notified Intel, and gave the users a temporary workaround.
  - The team made a small change in the I/O routine of a climate code from Goddard, and improved its writing performance by a factor of five.
  - The team identified and provided a fix for a page cache issue that was causing crashes in an application used by the GRAIL project.
  - The team worked with an OVERFLOW user from Ames whose code additions were performing poorly. Coaching him on how the application achieves load balance resulted with a nearly three-fold improvement.
- The APP team also improved its Lumber tool to provide information about the applications and libraries used in jobs. The myNAS web page team is using Lumber data to provide near-real-time feedback on jobs to PIs, users, and managers.

Mission Impact: The Application Performance and Productivity team enables researchers to better utilize NASA's supercomputing resources for their modeling and simulation projects supporting the agency's mission and goals.

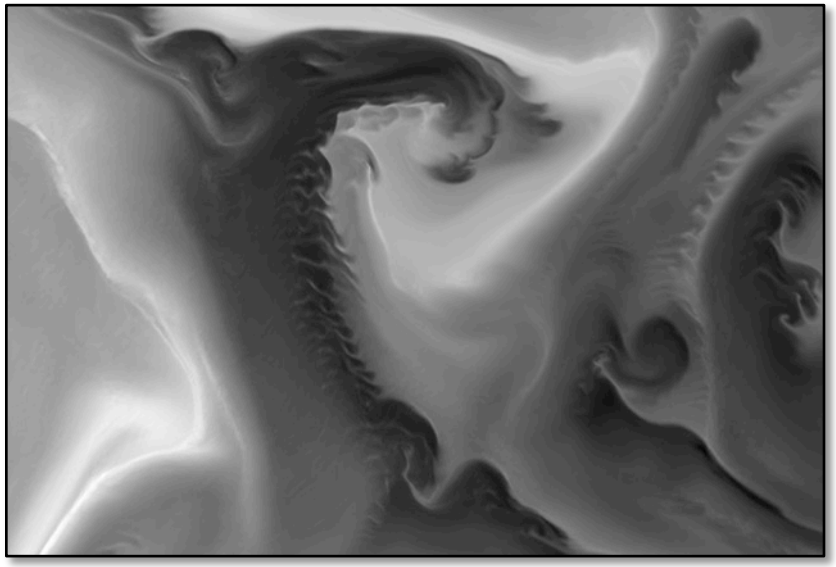
The Application Performance and Productivity team provides a variety of services aimed at allowing users to maximize the use of their allocations on HECC resources. The services include: helping with application issues, code optimization, system benchmarking, and tool development.

POCs: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165, NASA Advanced Supercomputing (NAS) Division;
Robert Hood, robert.hood@nasa.gov, (650) 604-0740, NAS Division, CSRA LLC

HECC Supercomputer Usage in April 2017 Sets New Record of Nearly 25 Million SBUs

- In April, the combined usage on HECC supercomputers set a new record of 24,856,653 Standard Billing Units (SBUs*).
- Usage of Pleiades, Electra, Merope, and Endeavour by 330 science and engineering projects from across NASA contributed to this record.
- Usage exceeded last month's (March 2017) by more than 373,000; and exceeded the January 2017 record by more than 2 million.
- This increase was enabled by high demand, system stability, and efficient operations. Electra and Pleiades both delivered system utilization of over 90% (75% is the target).
- The top 10 projects used between 402,448 and 2,520,858 SBUs, and accounted for over 39% of the total usage.
- The HECC Project continues to plan and evaluate ways to address the future requirements of NASA's users.

Mission Impact: Increasing capacity of HECC systems provides Mission Directorates with more resources to accomplish their goals and objectives.



Snapshot from an ultra-high-resolution visualization produced for the Estimating the Circulation and Climate of the Ocean (ECCO) project in support of NASA's Surface Water and Ocean Topography (SWOT) altimetry mission. ECCO was among the top 10 in HECC resource usage for April 2017. *Chris Henze, NASA/Ames*

POC: Blaise Hartman, blaise.hartman@nasa.gov, (650) 604-2539, NASA Advanced Supercomputing Division, CSRA LLC

** 1 SBU equals 1 hour of a Pleiades Westmere 12-core node.*

ESS Team Rolls Out Mac FileVault Password Enforcement

- HECC's Engineering Servers and Services (ESS) team previously deployed a FileVault (boot account) password change capability, but relied on users to change their passwords. New code was developed to enforce changing this FileVault password.
- The solution developed has two parts:
  - "Notification" periodically checks FileVault password ages and prompts users to change expiring passwords.
  - "Enforcement" takes place when an expired FileVault password is detected. If management approves locking the system, it is immediately locked and the user is unable to log in without system administrator assistance. Requiring management approval prevents automatic locking of a system when the user might be offsite and unable to recover.
- Password change information is also saved to an online database to facilitate automated notification to administrators and security.

Mission Impact: FileVault password enforcement ensures that users change their boot account passwords every 60 days as required by NASA regulations.

The "Boot Password Update" application, developed by the HECC Engineering Servers and Services team, identifies users' last successful password change, and is used for changing FileVault passwords.

POC: Ted Bohrer, theodore.w.bohrer@nasa.gov, (650) 604-4335, NASA Supercomputing Division, ADNET Systems

Apple's macOS 10.12 Sierra Deployed to Staff Workstations

- The HECC Engineering Servers and Services (ESS) team completed development of a Sierra image to deploy on about 200 Mac systems used by staff at the NAS facility.
- Once the image passed a NAS security scan and was approved by the NASA Ames security official, the ESS team began deployment to beta users to further validate the image.
- Preparation work for the Sierra rollout included: creating disk and netboot images; configuring settings to meet security and interoperability requirements; setting up configuration enforcements in Jamf Pro and CFEngine; testing all software; and overcoming issues with Centrify.
- Scripted configurations using Jamf Pro provided more automation and a shortened upgrade time as compared to OS X 10.11.

Mission Impact: Apple's annual release of a major operating system (OS) makes it a challenge for enterprise sites to stay current and run the latest OS. The Sierra upgrade allows HECC to provide the latest OS and hardware to scientific users and staff.

Apple's macOS 10.12 Sierra released on September 20, 2016, and is required for the latest MacBook Pro laptops.

POC: Edmund Garcia, edmund.a.garcia@nasa.gov, (650) 604-1338, NASA Advanced Supercomputing Division, ADNET Systems

HECC Supercomputing: A Superhero of NASA Science & Engineering at Silicon Valley Comic Con

- A team of HECC researchers, administrators, and support staff organized and produced a successful outreach exhibit in the NASA booth at Silicon Valley Comic Con, held April 21–23 in San Jose, CA.
- The exhibit was featured as part of the extensive NASA presence at the event, and the HECC team greeted thousands of attendees who were excited to talk to experts about the role of supercomputing and modeling & simulation across the agency's missions.
- Visitors were drawn into the exhibit by a video showing an animated fly-through of the NASA Advanced Supercomputing (NAS) Division facility and Pleiades supercomputer, as well as compelling visualizations from simulations representing research from several mission directorates. Simulations included:
  - Evolution of giant, turbulent molecular clouds.
  - Magnetic fields carpeting the sun.
  - The Space Launch System launch pad environment.
  - Complex rotor blade aerodynamics.
- HECC Deputy Project Manager Bill Thigpen and NAS Division researchers Mike Rogers and Stu Rogers participated in the "NASA in Silicon Valley: Technology of the Future" panel; their discussion of HECC's new modular supercomputing facility and their latest research drew applause from a capacity crowd.

Mission Impact: NASA's exhibit at Silicon Valley Comic Con provided an excellent public outreach opportunity to highlight the critical role of HECC resources in science and engineering projects across the agency.

Top: Bond Nguyen (left) and Chris Mattenberger staff the HECC exhibit at the NASA booth at Silicon Valley Comic Con. Bottom: HECC Deputy Project Manager Bill Thigpen (far right) and NAS Division researchers Mike Rogers (second from left) and Stu Rogers (middle) participate in the "NASA in Silicon Valley: Technology of the Future" panel.

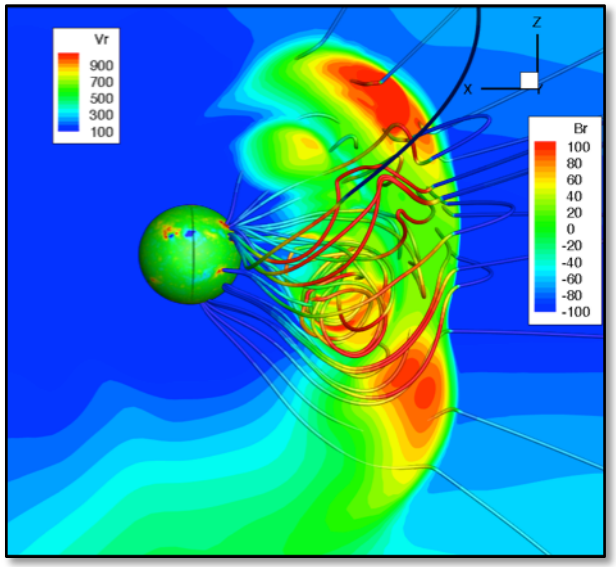
POC: Michelle Moyer, michelle.c.moyer@nasa.gov, (650) 604-2912, NASA Advanced Supercomputing Division, CSRA LLC

Simulating the Propagation of Coronal Mass Ejections Through the Heliosphere *

- Researchers ran simulations on Pleiades to study coronal mass ejections (CMEs) – powerful expulsions of plasma from the sun that interact with Earth's magnetosphere, causing "space weather."
  - Using the Space Weather Modeling Framework global magnetohydrodynamics code, the researchers ran CME propagation simulations initiated by a realistic, 3D nonlinear force-free magnetic field model of a solar active region that erupted on April 8, 2010.
  - 3D variables of plasma parameters (velocity, density, temperature, and magnetic field) were produced as a function of position and time, as well as simulated white light and extreme ultraviolet emissions that have been observed by space-based telescopes.
  - The model that best matched observations had axial flux of 11 x 1,020 maxwells (units of magnetic flux) and produced a CME velocity of 740 kilometers per second.
- This project presented the most realistic CME propagation simulations produced to date, and has the potential to increase the ability of such simulations to help predict space weather.
- Each simulation ran for 16 days or more using at least 1,000 Pleiades cores; the project currently stores 6.5 terabytes of data on HECC systems.

** HECC provided supercomputing resources and services in support of this work.*

Mission Impact: Enabled by HECC resources, this project supports NASA's goal to improve space weather forecasts by helping researchers learn to predict where, when, and how coronal mass ejections originate and how they propagate through the heliosphere.



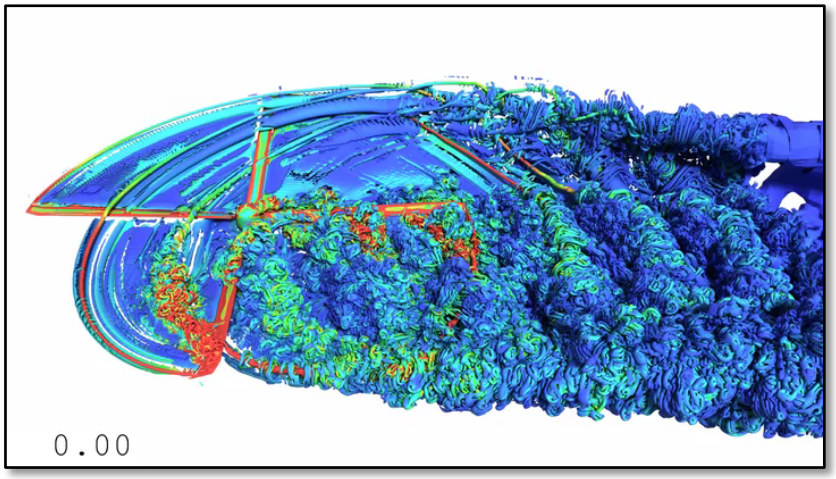
Coronal mass ejection (CME) propagation simulation showing sample magnetic field lines through the CME ejecta 1:05 hours after the start of an eruption.

POC: Antonia Savcheva, asavcheva@cfa.harvard.edu, (617) 495-7121, NASA Ames Research Center, Harvard-Smithsonian Center for Astrophysics

Researchers Gain New Insights Into Dynamic Stall for High Performance Helicopters *

- Researchers at NASA Ames used the OVERFLOW CFD code to study the effects of adaptive mesh refinement (AMR) on the vortex wake of an isolated helicopter rotor during blade-vortex interactions (BVI) and dynamic stall events. BVI can cause unacceptable noise levels; dynamic stall limits a helicopter's lifting capability and maximum flight speed.
- The study revealed some surprising results:
  - The predicted aerodynamic loads did not depend on refining the rotor wake beyond what is normally done for engineering calculations—good news for design engineers who must compute many CFD simulations on coarser grids to reduce analysis time and cost.
  - Vortices passing over the top of rotor blades triggered dynamic stall. It was previously thought that a rotor blade pitching up to a high angle of attack was the sole cause of dynamic stall.
- Time-dependent flow visualization was crucial to understanding the relationship between blade-tip vortices and dynamic stall.
- Researchers are now exploring the use of AMR on the rotor blades rather than the rotor wake.

Mission Impact: Enabled by the Pleiades supercomputer and HECC storage capabilities, CFD simulations provide greater insight and improved prediction accuracy for blade-vortex interaction, to help NASA's Revolutionary Vertical Lift Technology project increase helicopter performance and reduce noise levels and fuel consumption.



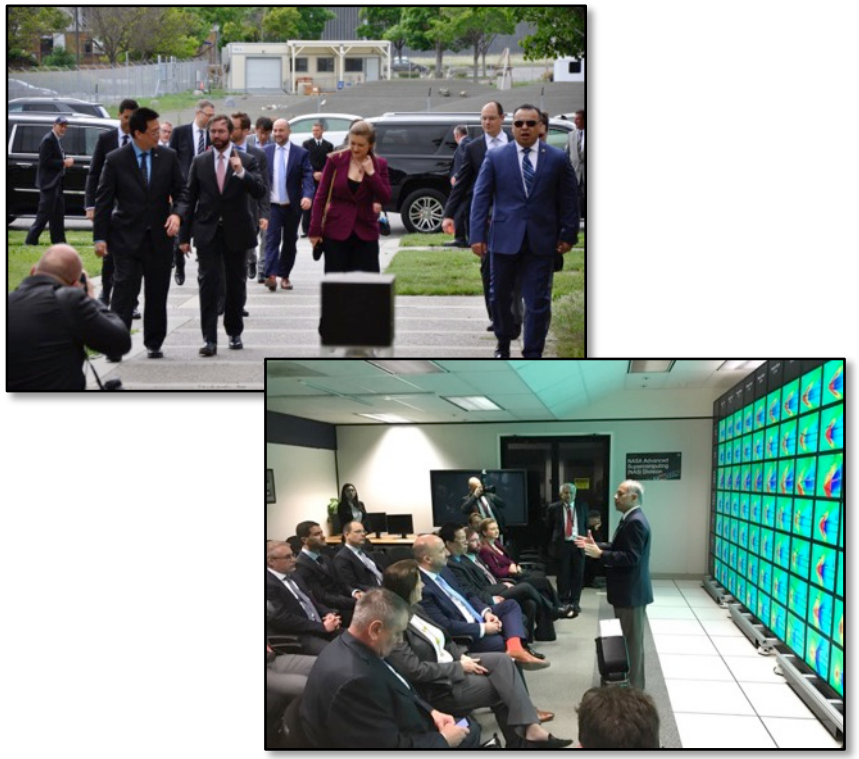
Video from simulation of dynamic stall for a Blackhawk helicopter rotor in forward flight. In this oblique view, the vortex wake is colored by vorticity magnitude (red is high, blue is low). *Tim Sandstrom, NASA/Ames*

POC: Neal Chaderjian, neal.chaderjian@nasa.gov, (650) 604-4472, NASA Advanced Supercomputing Division

** HECC provided supercomputing resources and services in support of this work.*

HECC Facility Hosts Several Visitors and Tours in April 2017

- HECC hosted 12 tour groups in April; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
  - A VIP delegation from Luxembourg visited the NAS facility this month, including the Crown Prince Guillaume; the Crown Princess Stéphanie; the Deputy Prime Minister, Etienne Schneider; the Ambassador of Luxembourg to the United States, Sylvie Lucas; and 10 other dignitaries. This group was accompanied by a media contingent of 30 people.
  - Thomas Zurbuchen, Associate Administrator for the Science Mission Directorate.
  - David McBride, Center Director at Armstrong Flight Research Center; with Deputy Center Director Patrick Stoliker and Chief of Staff Roberta Sherrard.
  - Greg Herrmann and Elise Murphy from Amazon's Security Office.



Top: Ames Center Director, Eugene Tu (left) escorts the Crown Prince Guillaume and the Crown Princess Stéphanie, along with a Luxembourg delegation and a media contingent, into the NAS facility. Bottom: Director of Exploration Technology at NASA Ames, Rupak Biswas (facing guests), NAS Division Chief Piyush Mehrotra (facing camera), and visualization specialist Tim Sandstrom presented HECC objectives and showed computational results on the NAS hyperwall to the Luxembourg guest.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers

- "**A Search for Lost Planets in the Kepler Multi-Planet Systems and the Discovery of the Long-Period, Neptune-sized Exoplanet Kepler-150f**," J. Schmitt, J. Jenkins, D. Fischer, The Astronomical Journal, vol. 153, no. 4, March 28, 2017. * *http://iopscience.iop.org/article/10.3847/1538-3881/aa62ad/meta*
- "**Plausible Compositions of the Seven TRAPPIST-1 Planets Using Long-term Dynamical Simulations**," B. Quarles, et al., arXiv:1704.02261 [astro-ph.EP], April 7, 2017. * *https://arxiv.org/abs/1704.02261*
- "**Influence of the North American Monsoon on Southern California Tropospheric Ozone Levels During Summer in 2013-2014**," M. Ganados-Muñoz, M. Johnson, T. Leblanc, Geophysical Research Letters, April 10, 2017. * *http://onlinelibrary.wiley.com/doi/10.1002/2017GL073375/full*
- "**Global Three-Dimensional Simulation of Earth's Dayside Reconnection Using a Two-Way Coupled Magnetohydrodynamics with Embedded Particle-in-Cell Model: Initial Results**," Y. Chen, et al., arXiv:1704.03803 [physics.space-ph], April 12, 2017. * *https://arxiv.org/abs/1704.03803*
- "**The Sensitivity of Rapidly Rotating Rayleigh-Bernard Convection to Ekman Pumping**," M. Plumley, et al., arXiv:1704.04696 [physics.flu-dyn], April 15, 2016. * *https://arxiv.org/abs/1704.04696*

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

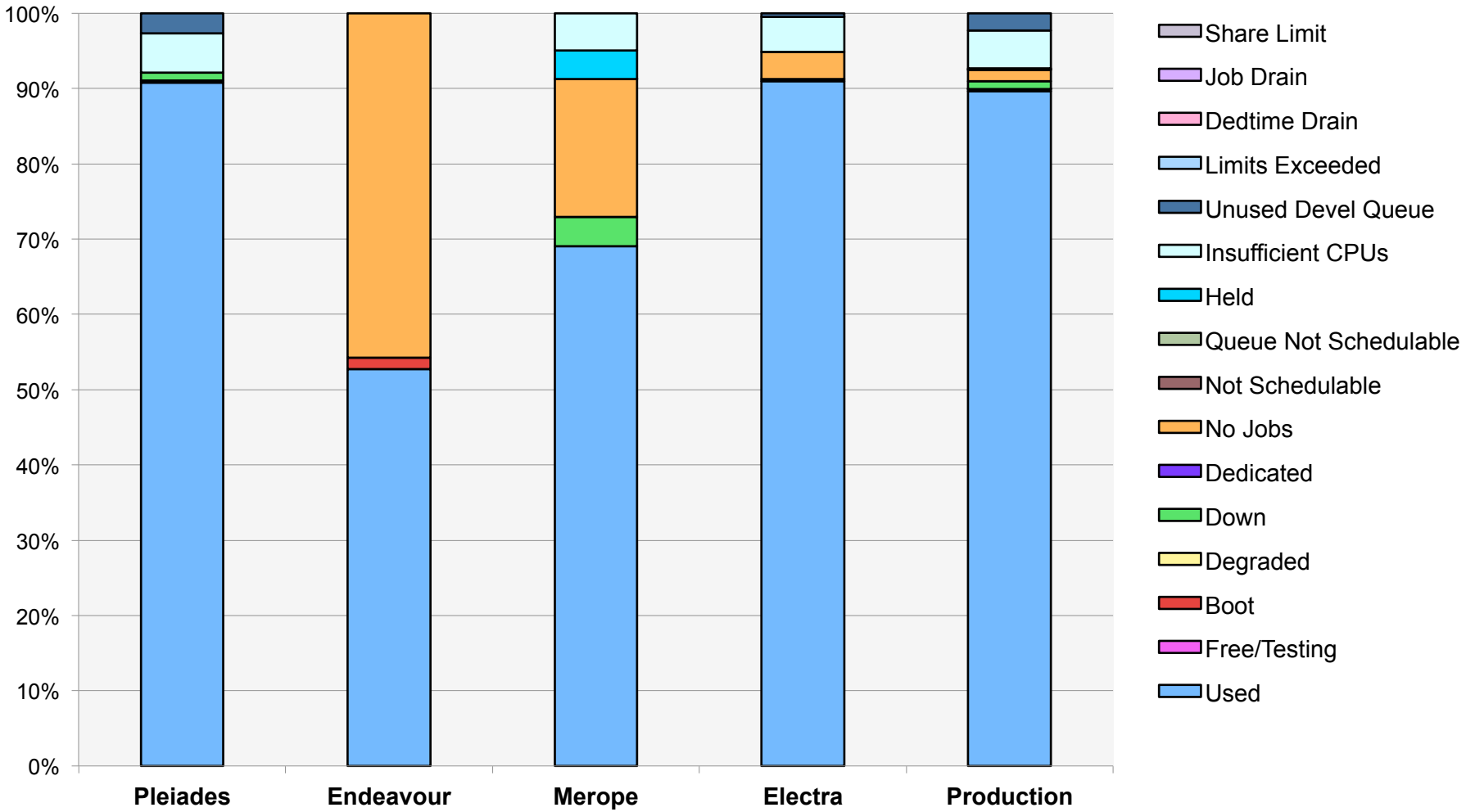
- "**T-Matrix and Radiative Transfer Hybrid Models for Densely Packed Particulates at Mid-Infrared Wavelengths**," G. Ito, J. Arnold, T. Glotch, Journal of Geophysical Research: Planets, April 18, 2017. *
  http://onlinelibrary.wiley.com/doi/10.1002/2017JE005271/full
- "**A Parameter Study for Modeling MgII h and k Emission During Solar Flares**," F. da Costa, L. Kleint, arXiv:1704.05874 [astro-ph.SR], April 19, 2017. *
  https://arxiv.org/abs/1704.05874
- "**Modeling Mangrove Propagule Dispersal Trajectories Using High-Resolution Estimates of Ocean Surface Winds and Currents**," T. Van der Stocken, D. Menemenlis, The Journal of the Association for Tropical Biology and Conservation (Biotropica), April 21, 2017. *
  http://onlinelibrary.wiley.com/doi/10.1111/btp.12440/full

** HECC provided supercomputing resources and services in support of this work*

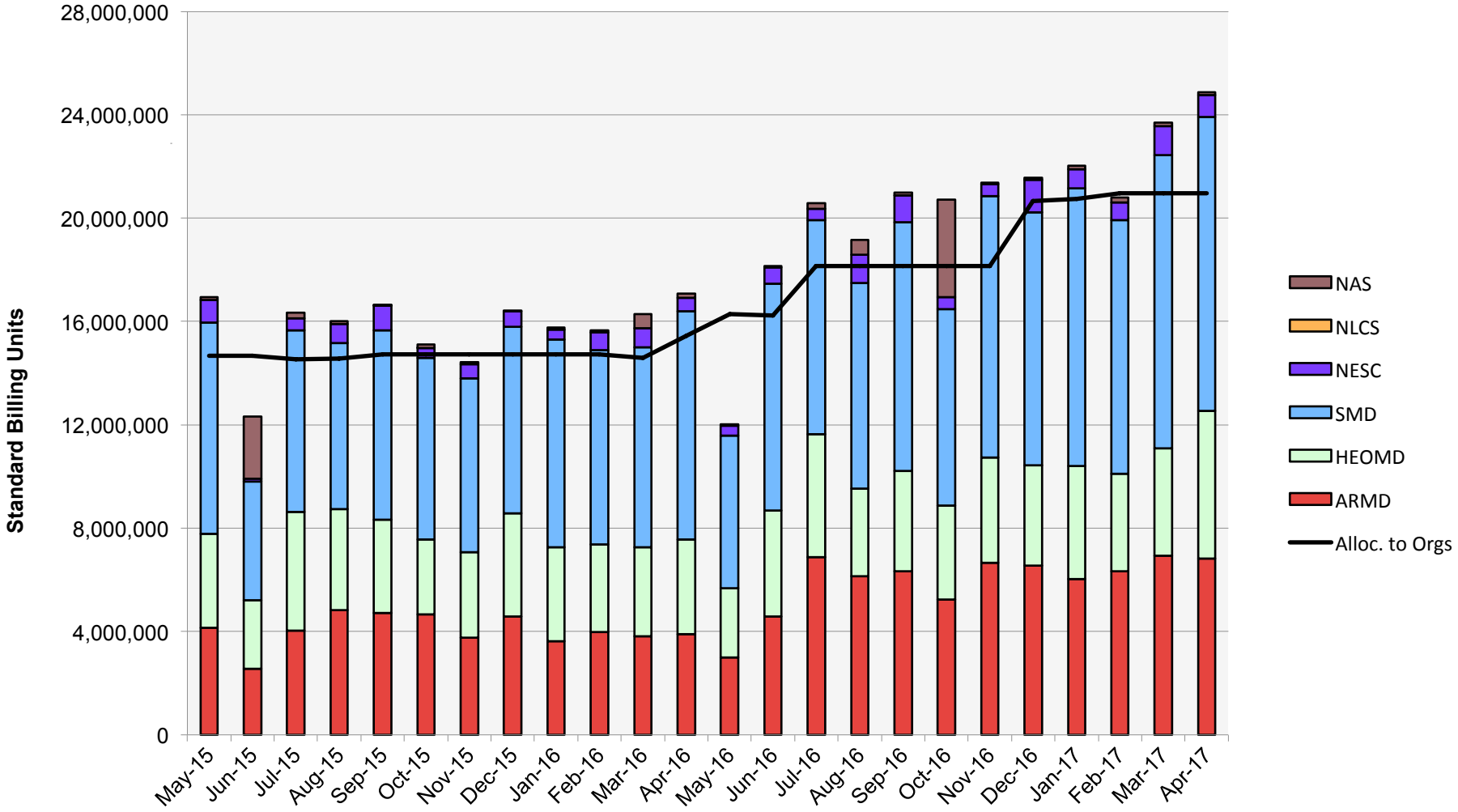
News and Events

- **NASA Ames at Silicon Valley Comic Con**, April 21-23, 2017—The NASA Advanced Supercomputing Division participated in the NASA exhibitors booth at the Silicon Valley Comic Con in San Jose, California. Volunteers from NAS greeted hundreds of attendees who were excited to speak to NASA experts about supercomputing at the agency. Additionally, Mike Rogers, Stu Rogers, and Bill Thigpen participated in the conference's "NASA in Silicon Valley: Technology of the Future" panel, in which they discussed Electra, which makes use of a new modular facility, and the modeling and simulation made possible by the division's computing and visualization resources. *http://svcomiccon.com/*
- **Photos: Super Heroes (and comic book fans) Unite in San Jose**, *Silicon Valley Business Journal,* April 23, 2017—Slide show including the "NASA in Silicon Valley: Technology of the Future" panel (see slide 9). *http://www.bizjournals.com/sanjose/news/2017/04/23/photossuper-heroes-and-comic-book-fans-unite-in.html*

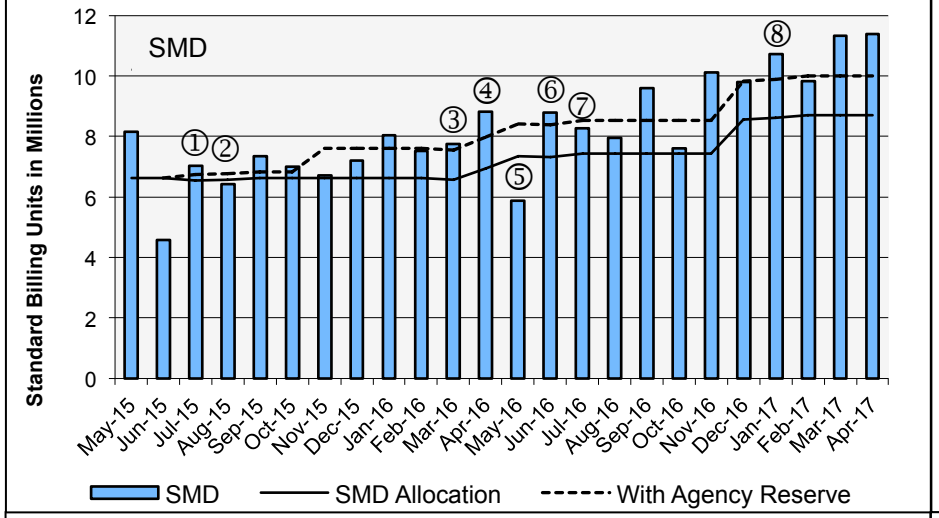
HECC Utilization

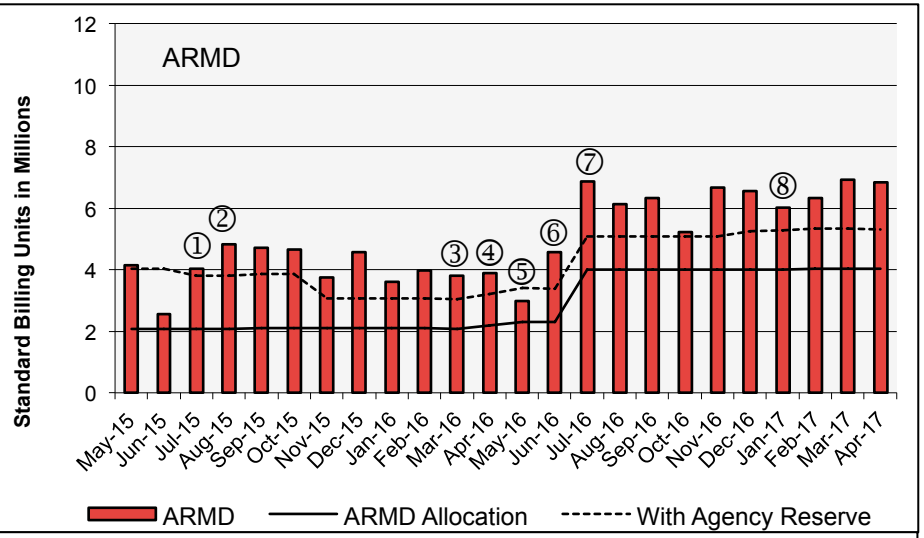


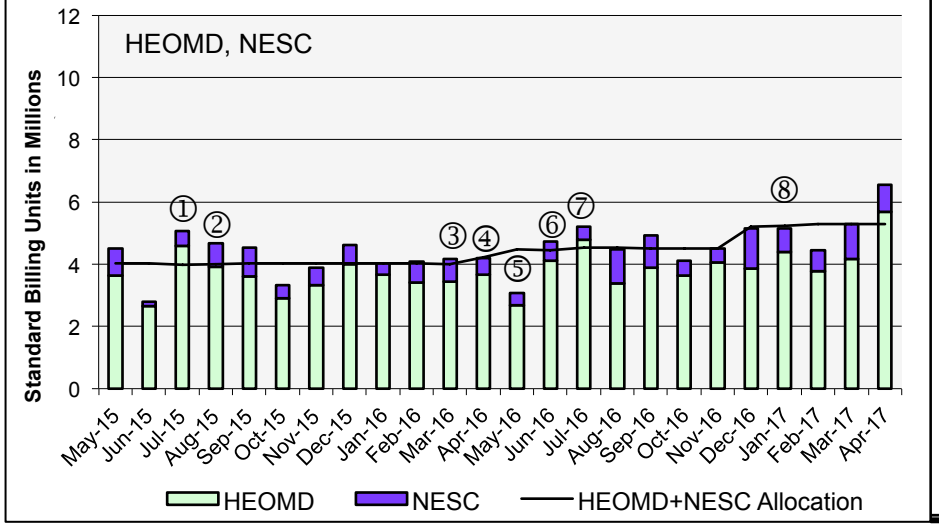
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month

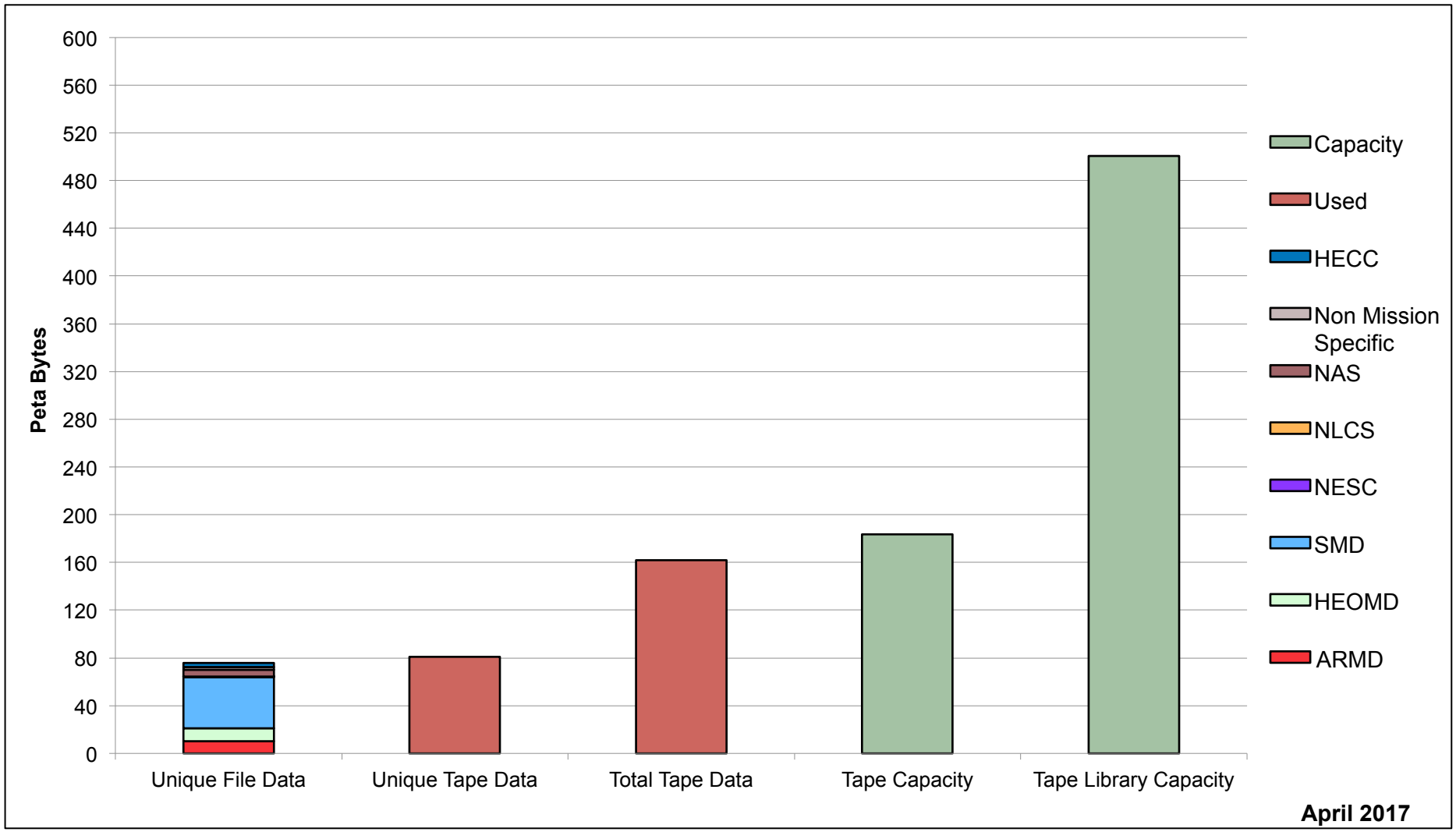






① 7 Nehalem ½ racks retired from Merope
② 7 Westmere ½ racks added to Merope
③ 16 Westmere racks retired from Pleiades
④ 10 Broadwell racks added to Pleiades
⑤ 4 Broadwell racks added to Pleiades
⑥ 14 (All) Westmere racks retired from Pleiades
⑦ 14 Broadwell Racks added to Pleiades
⑧ 16 Electra Broadwell Racks in Production, 20 Westmere 1/2 racks added to Merope

Tape Archive Status



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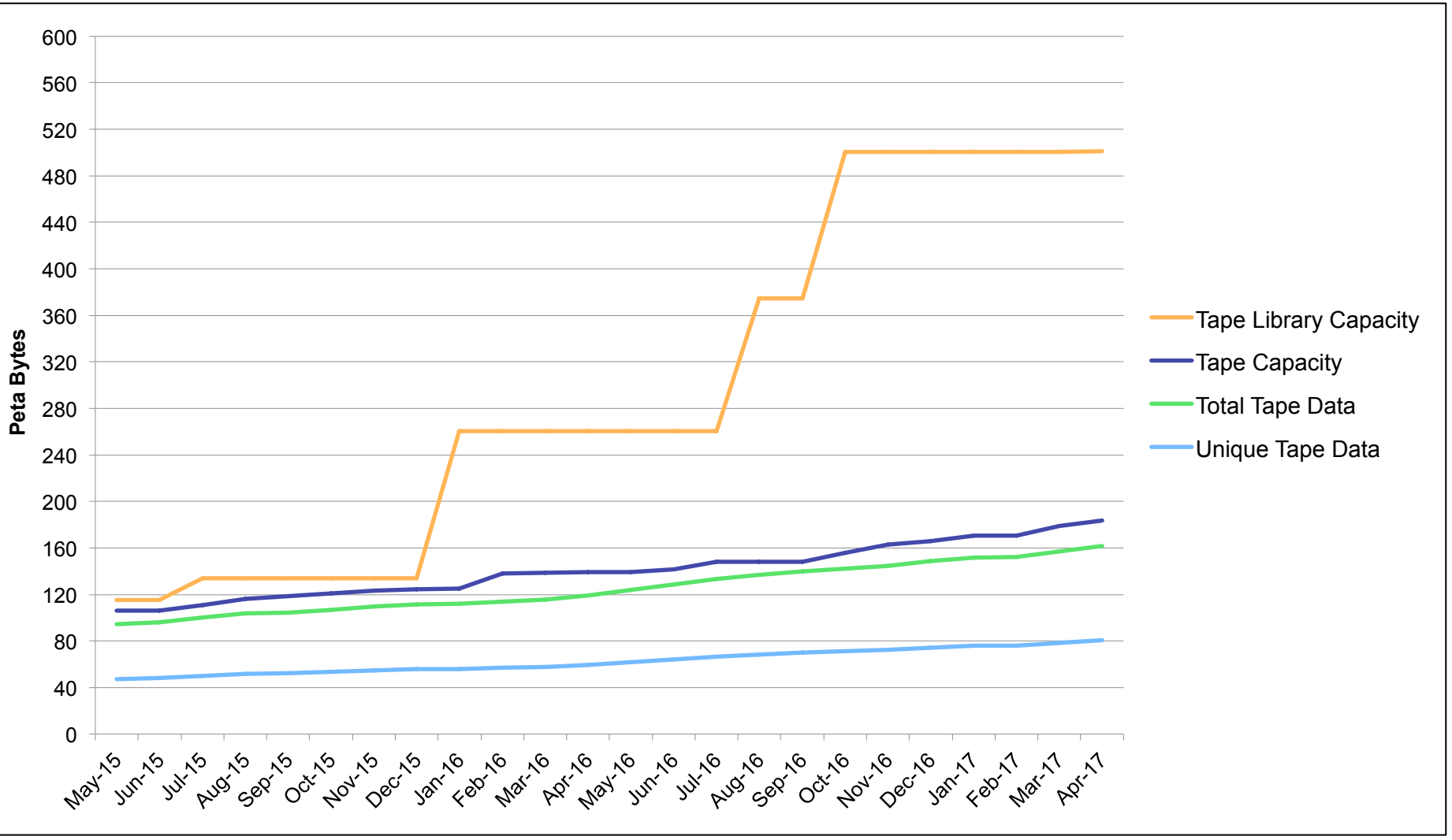
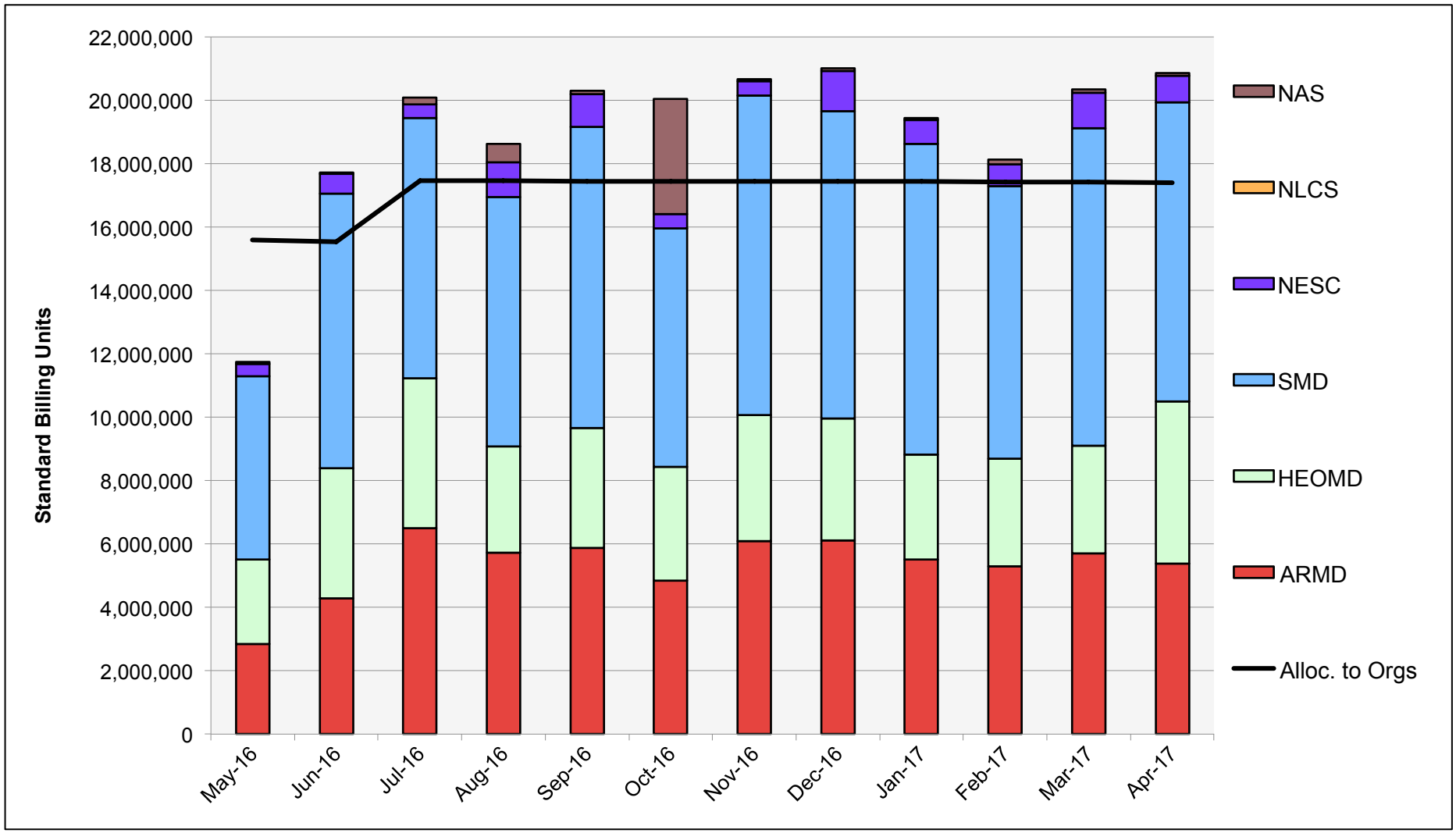
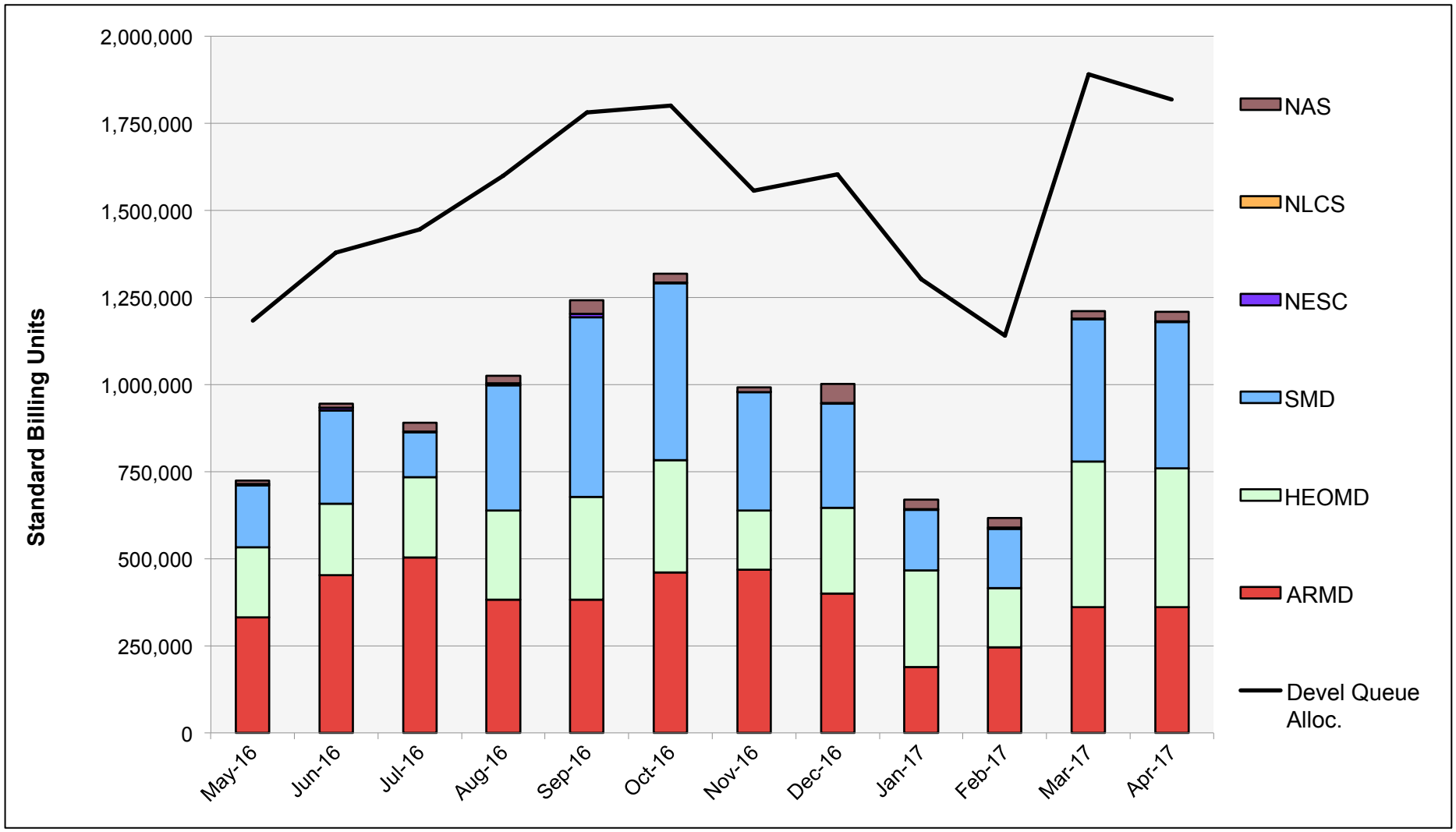


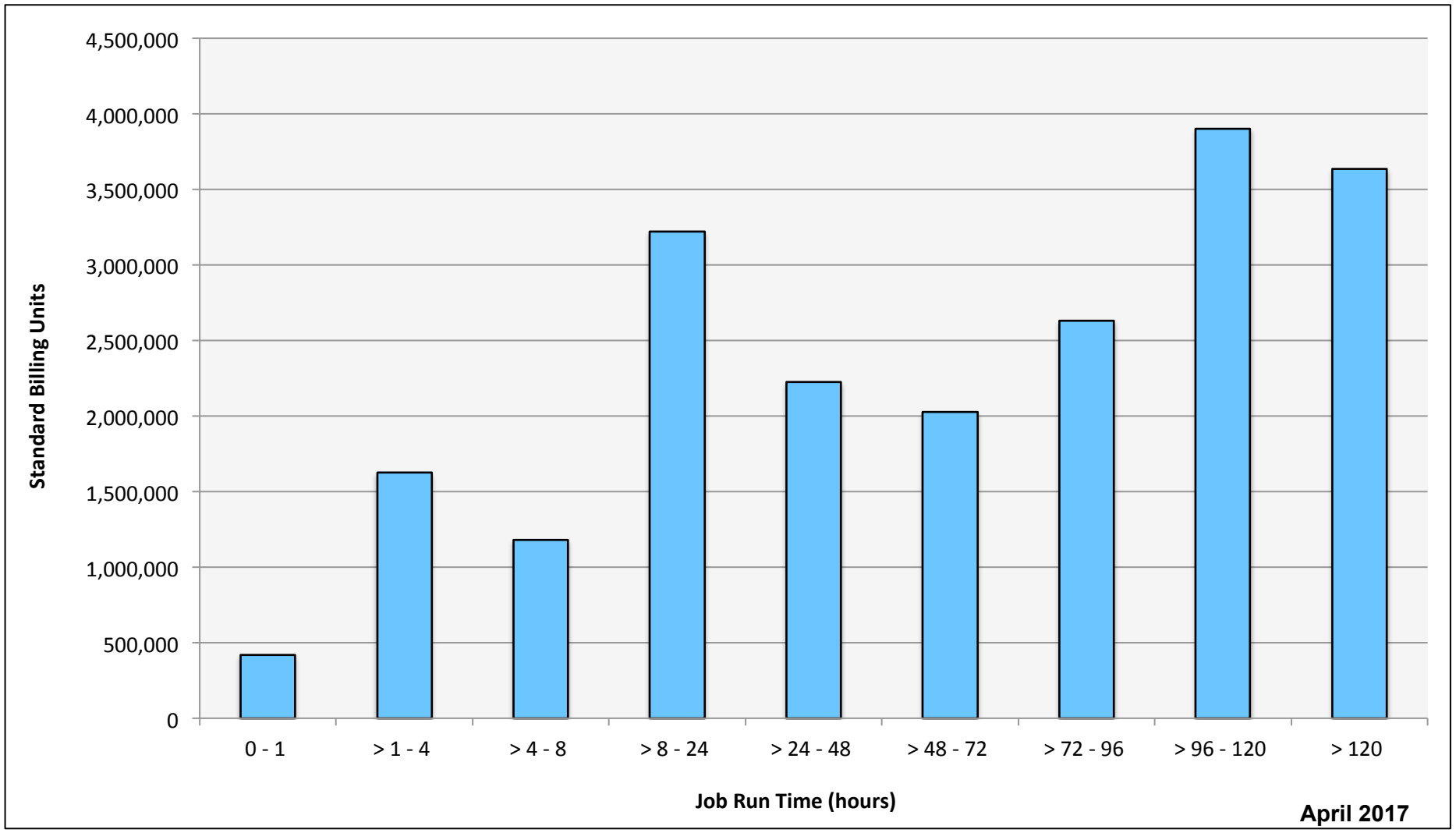
Pleiades:
SBUs Reported, Normalized to 30-Day Month



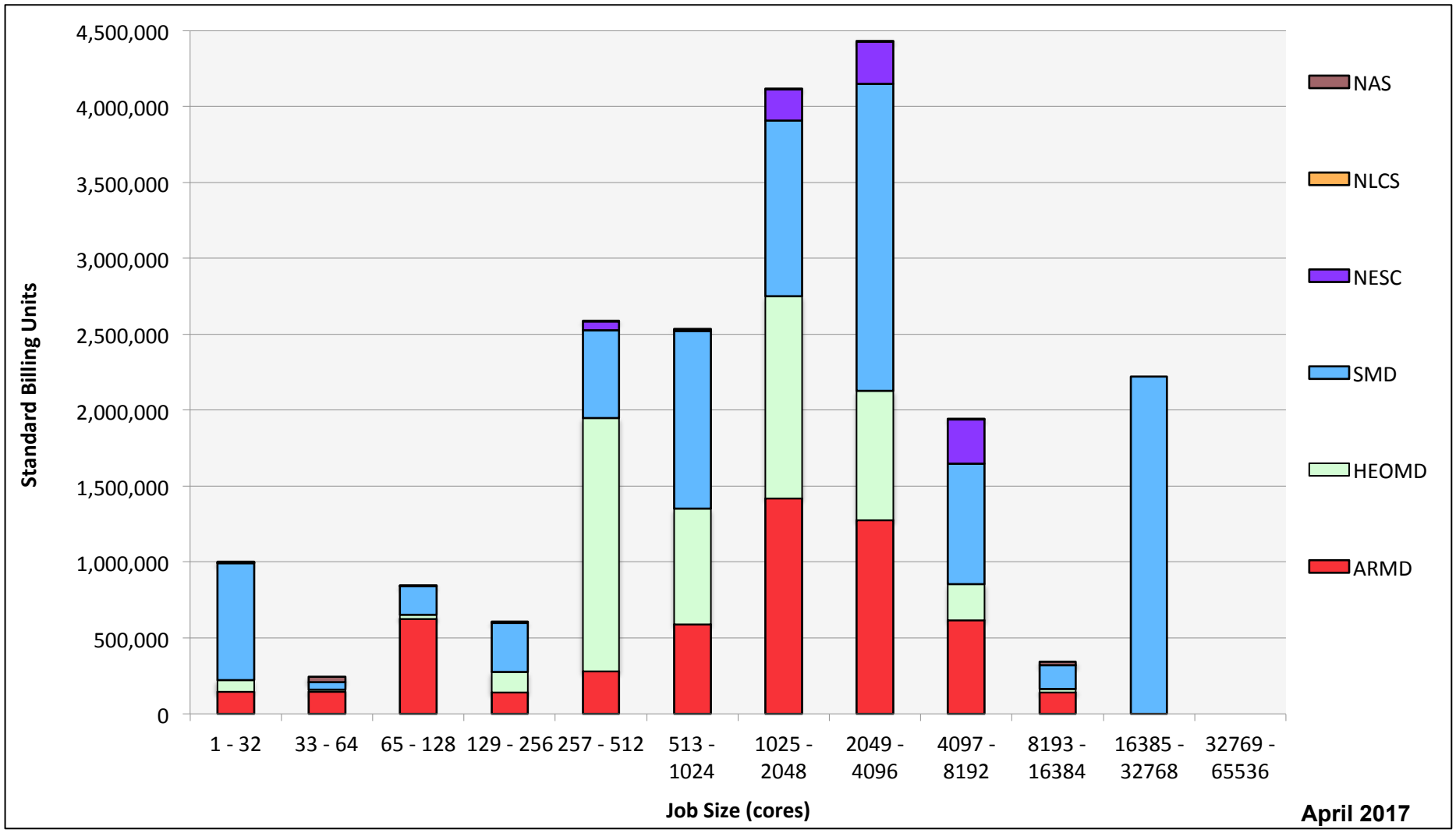
Pleiades:
Devel Queue Utilization



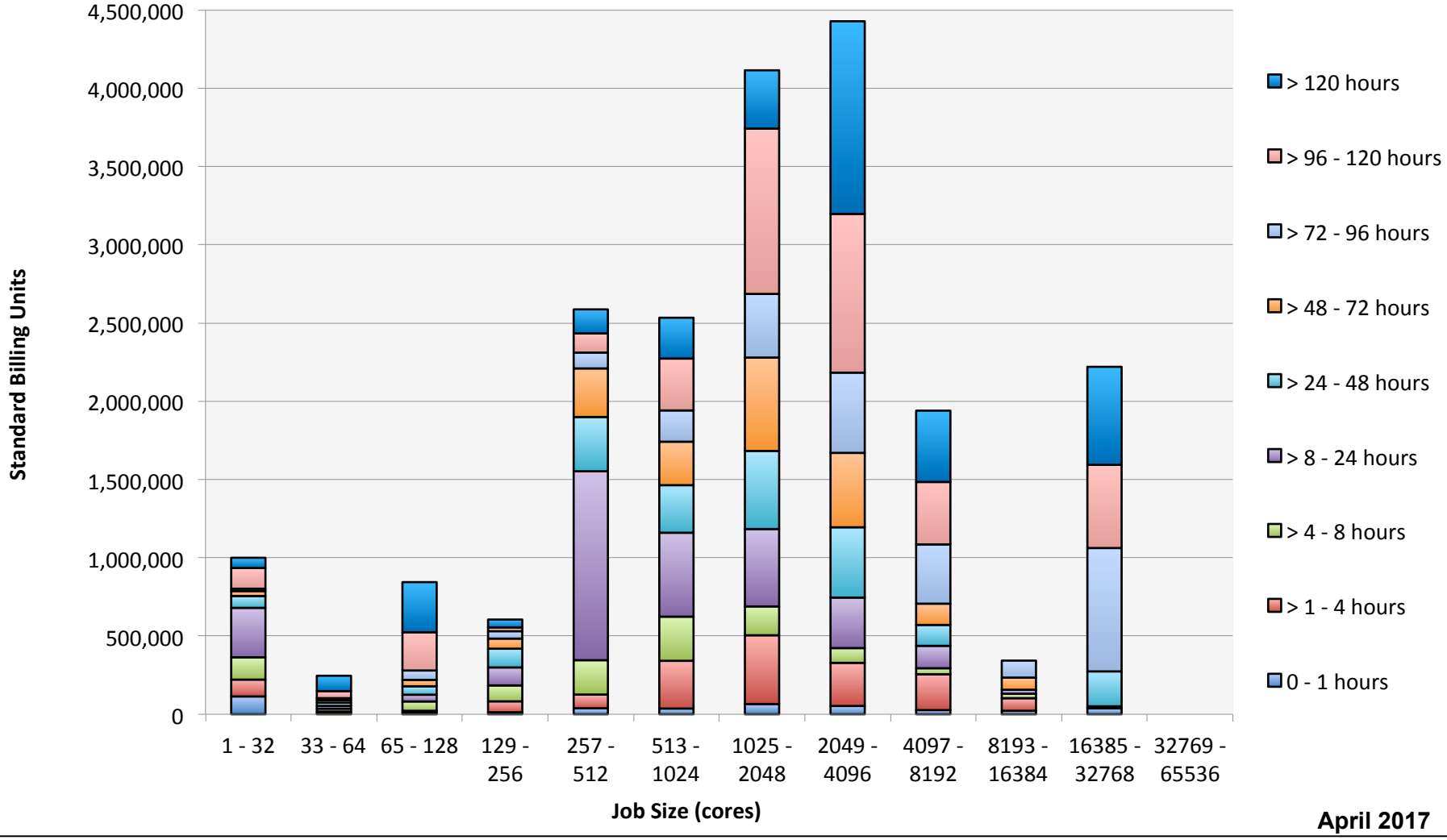
Pleiades:
Monthly Utilization by Job Length



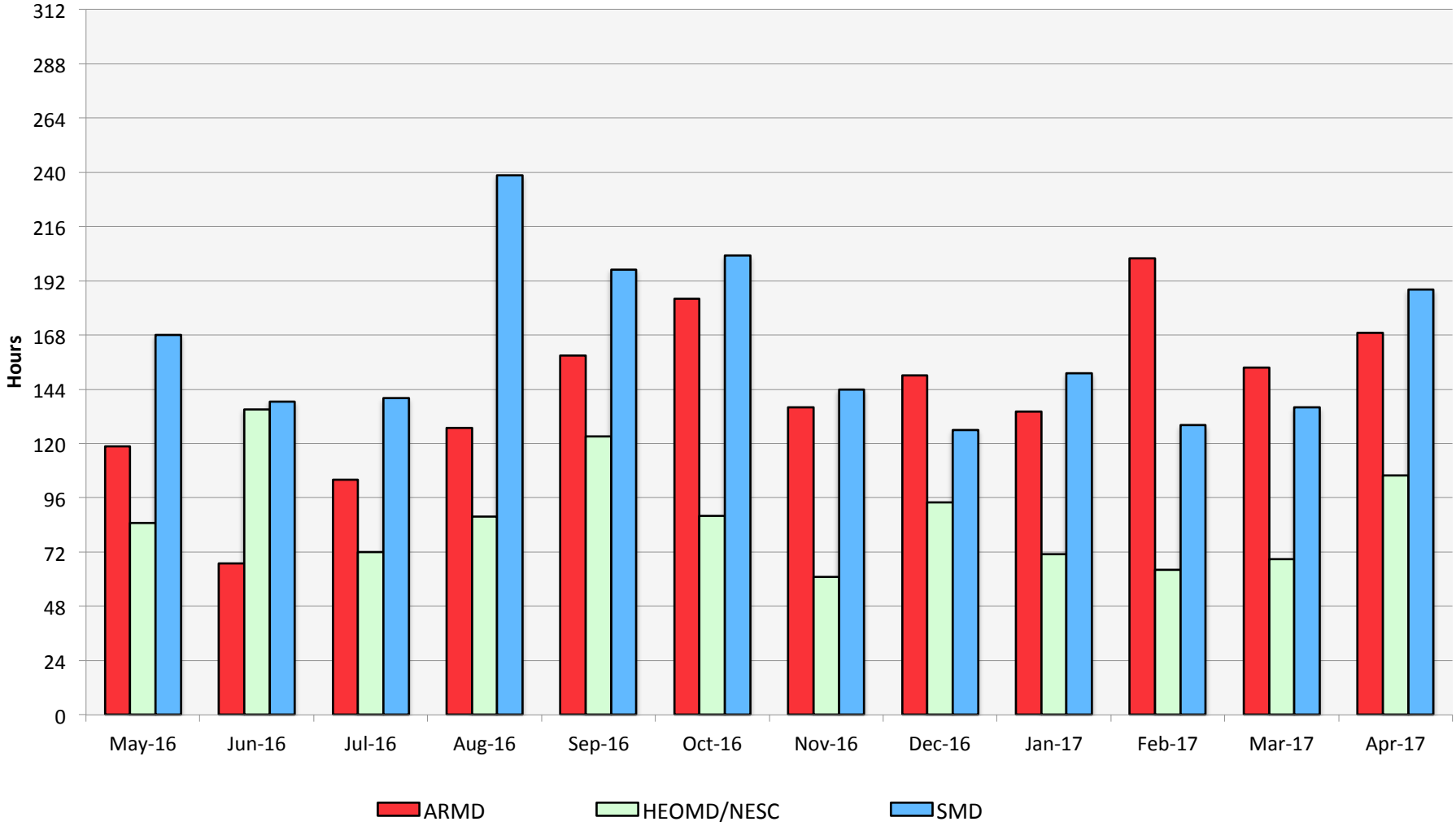
Pleiades:
Monthly Utilization by Size and Mission



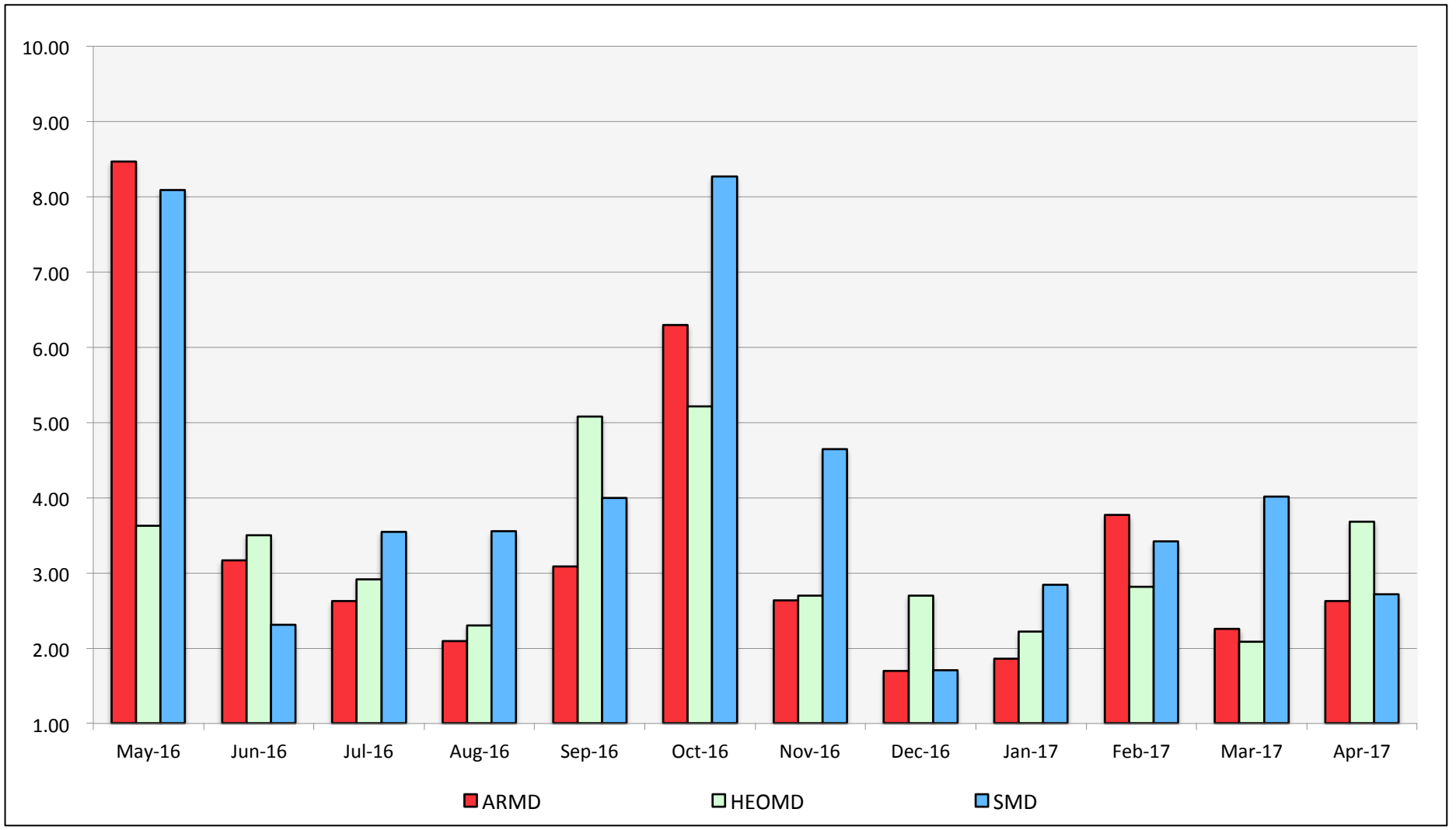
Pleiades:
Monthly Utilization by Size and Length



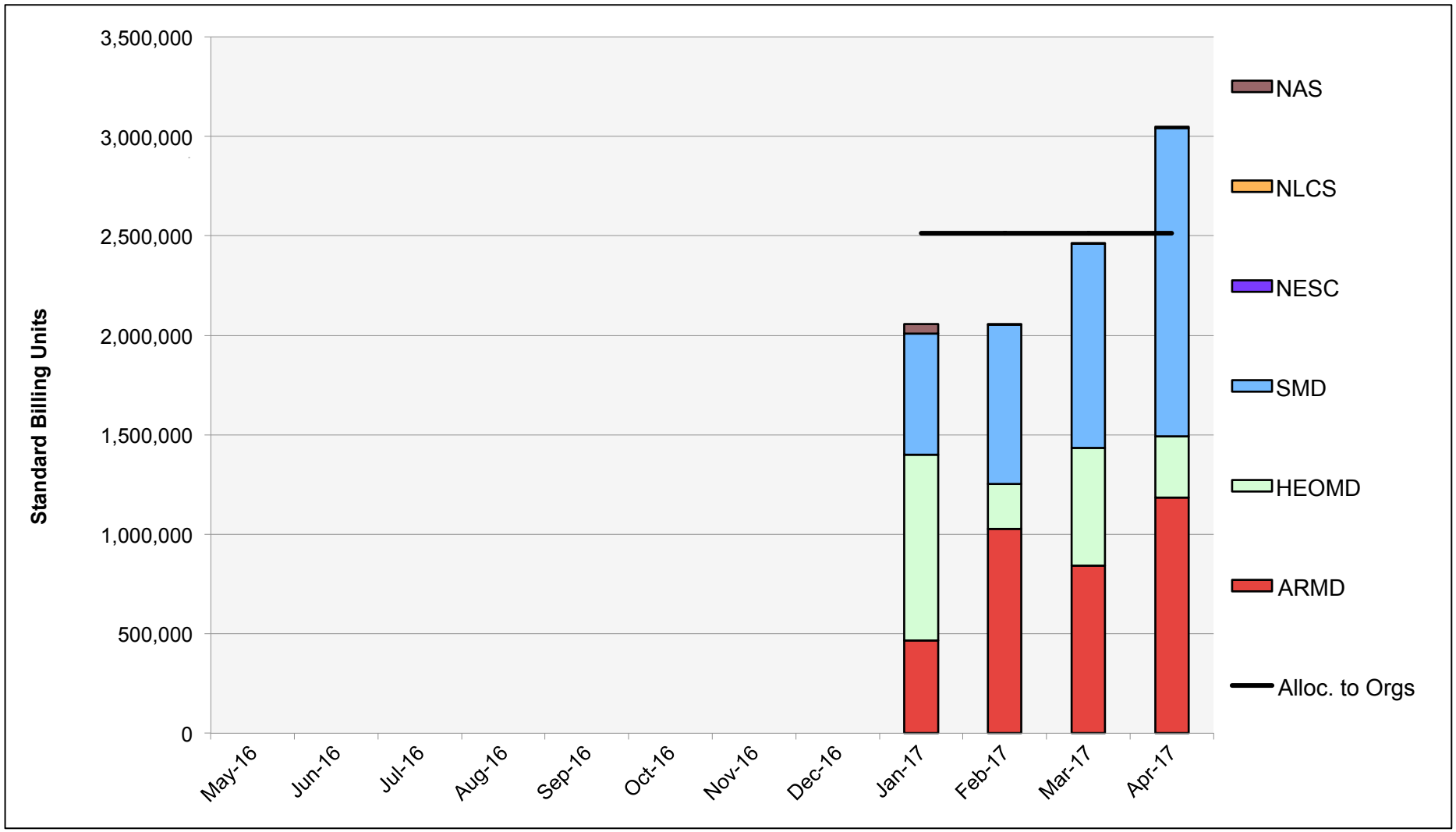
Pleiades:
Average Time to Clear All Jobs



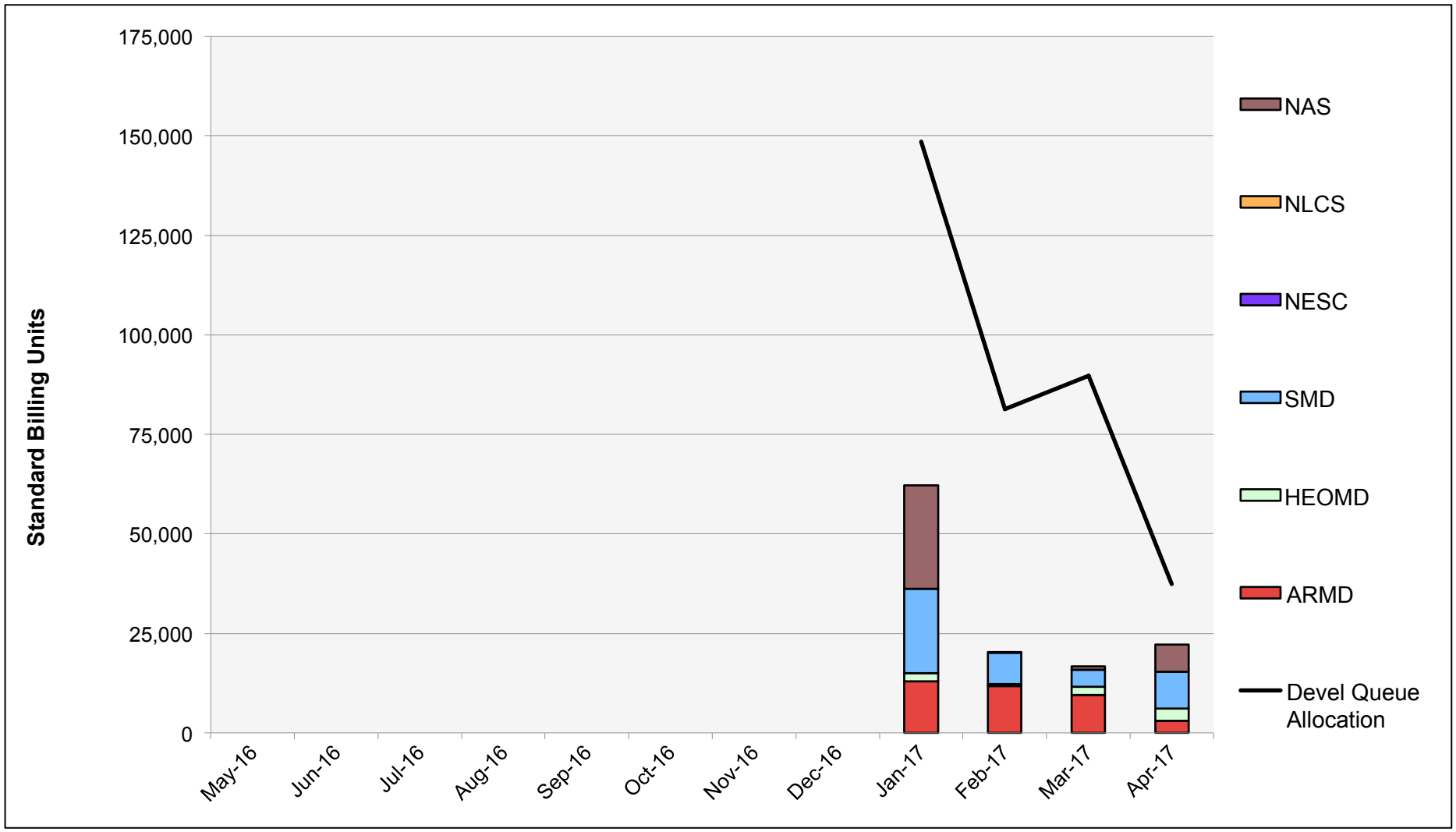
Pleiades:
Average Expansion Factor



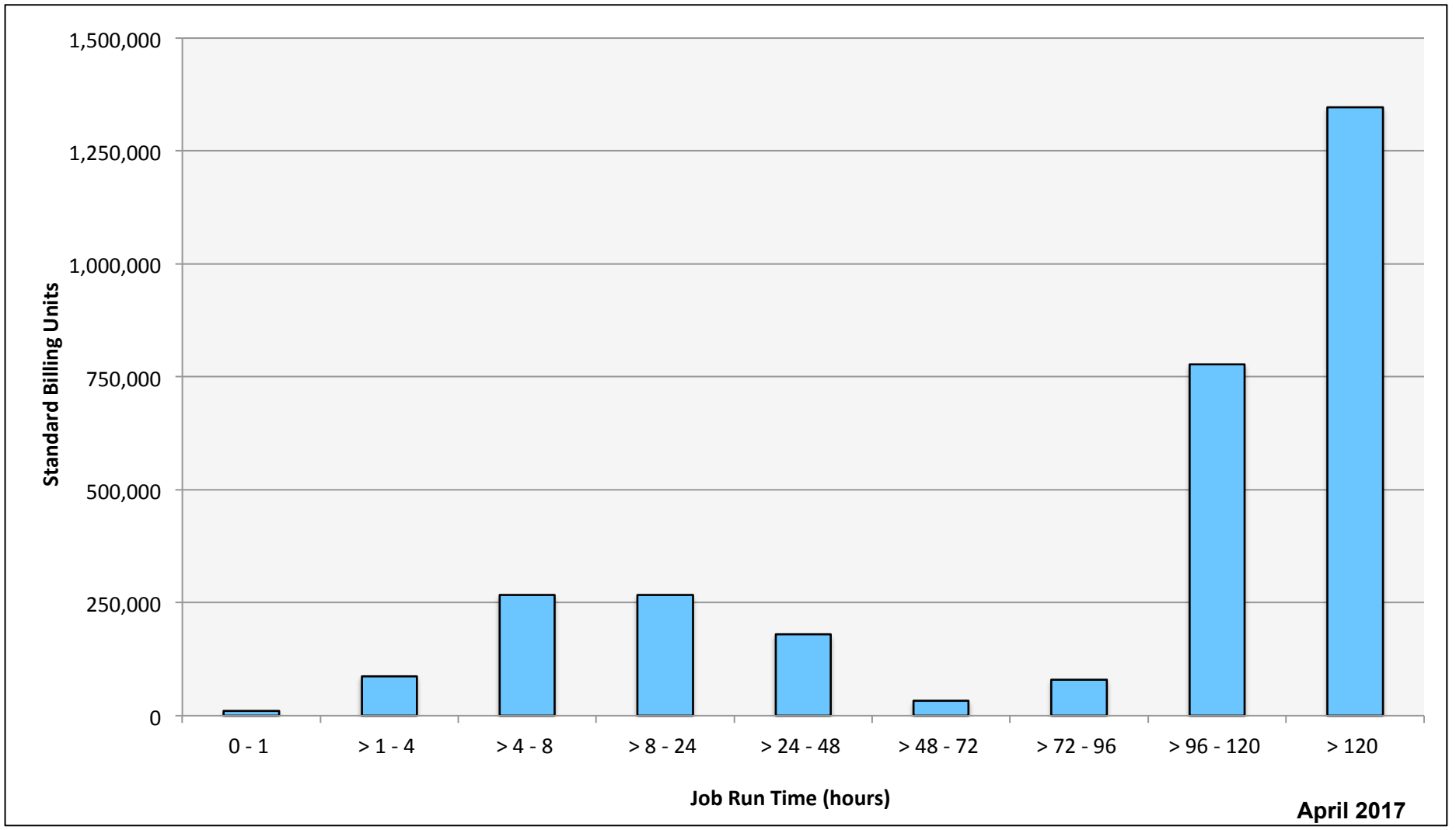
Electra:
SBUs Reported, Normalized to 30-Day Month



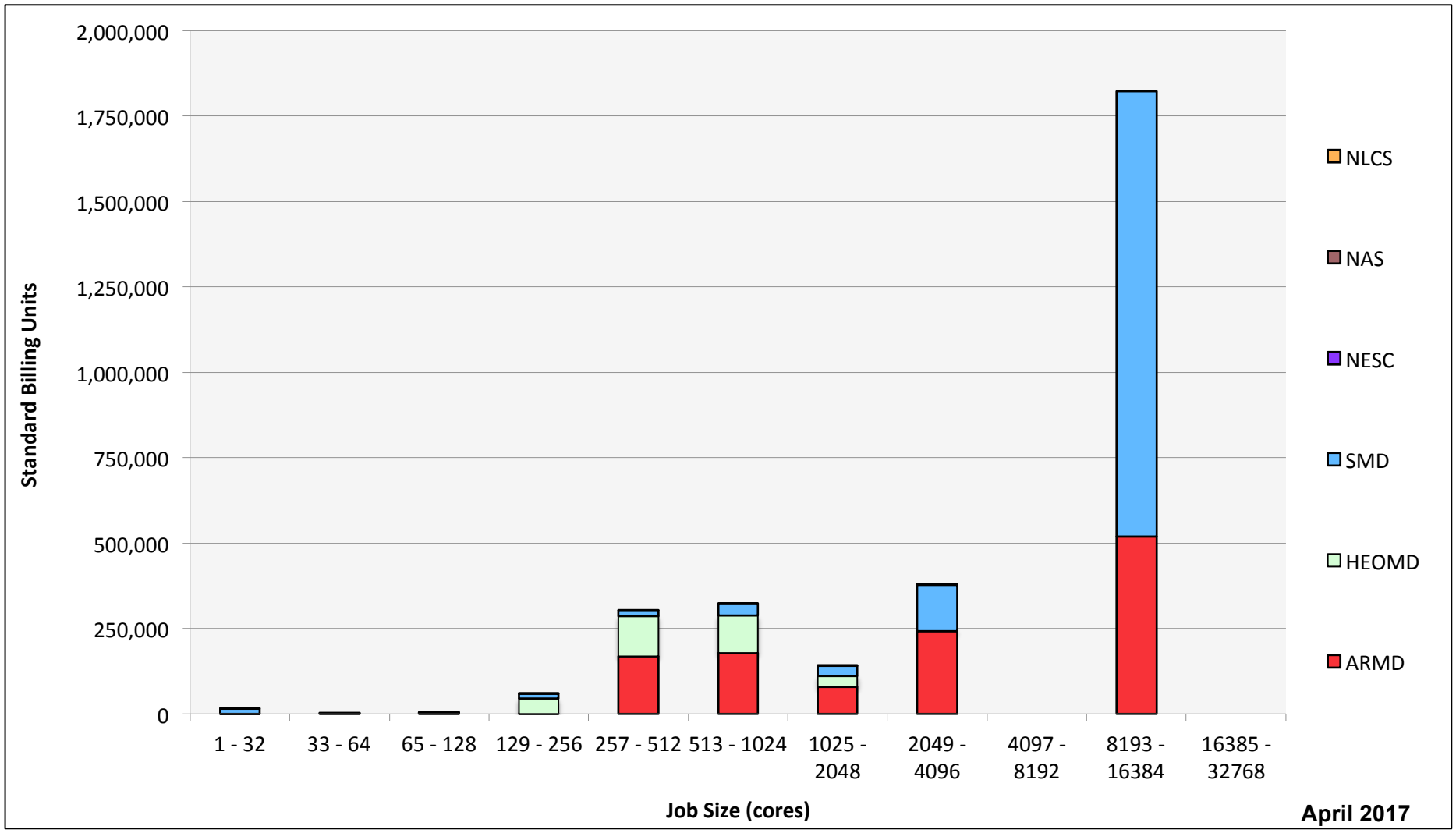
Electra:
Devel Queue Utilization



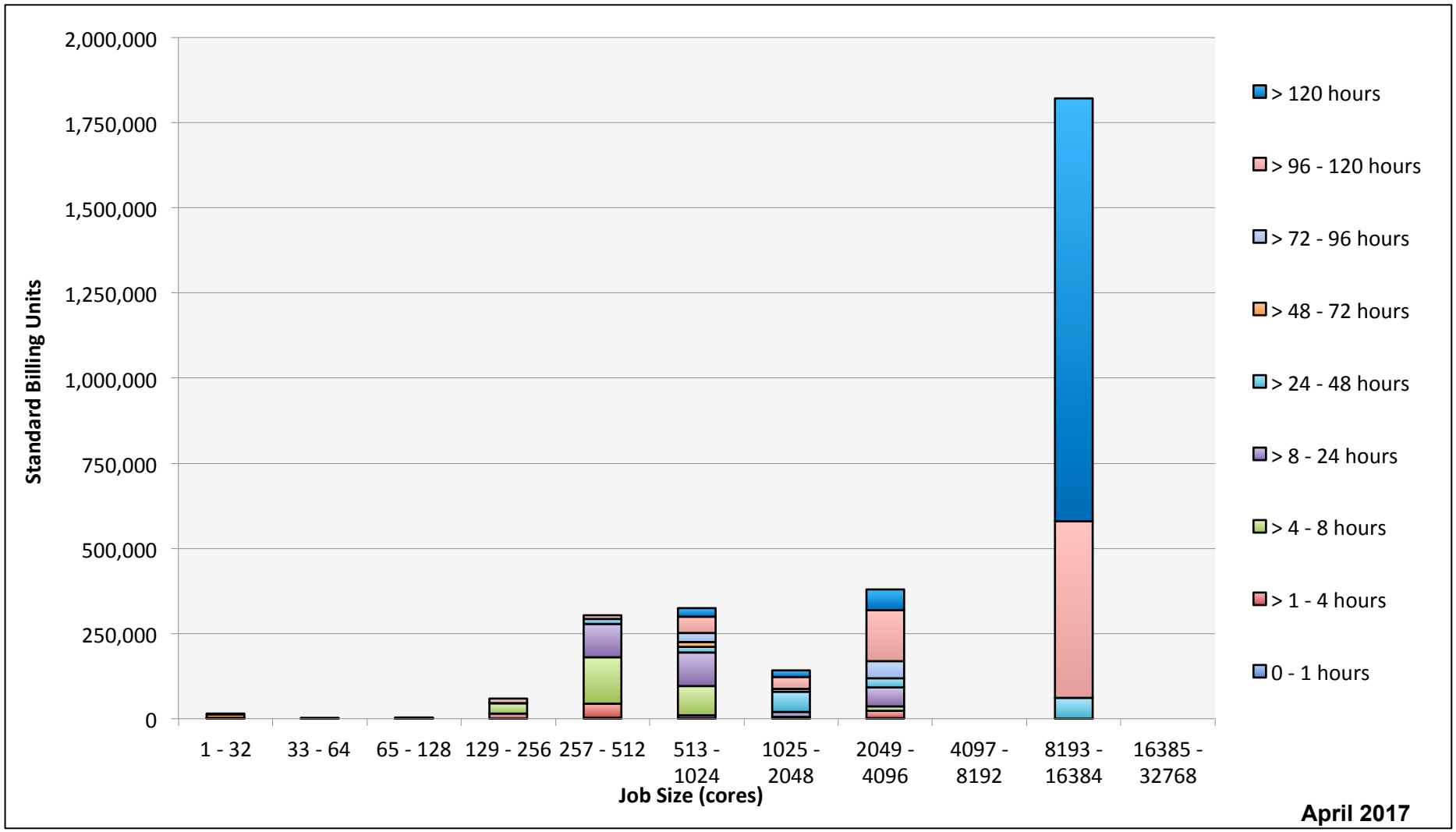
Electra:
Monthly Utilization by Job Length



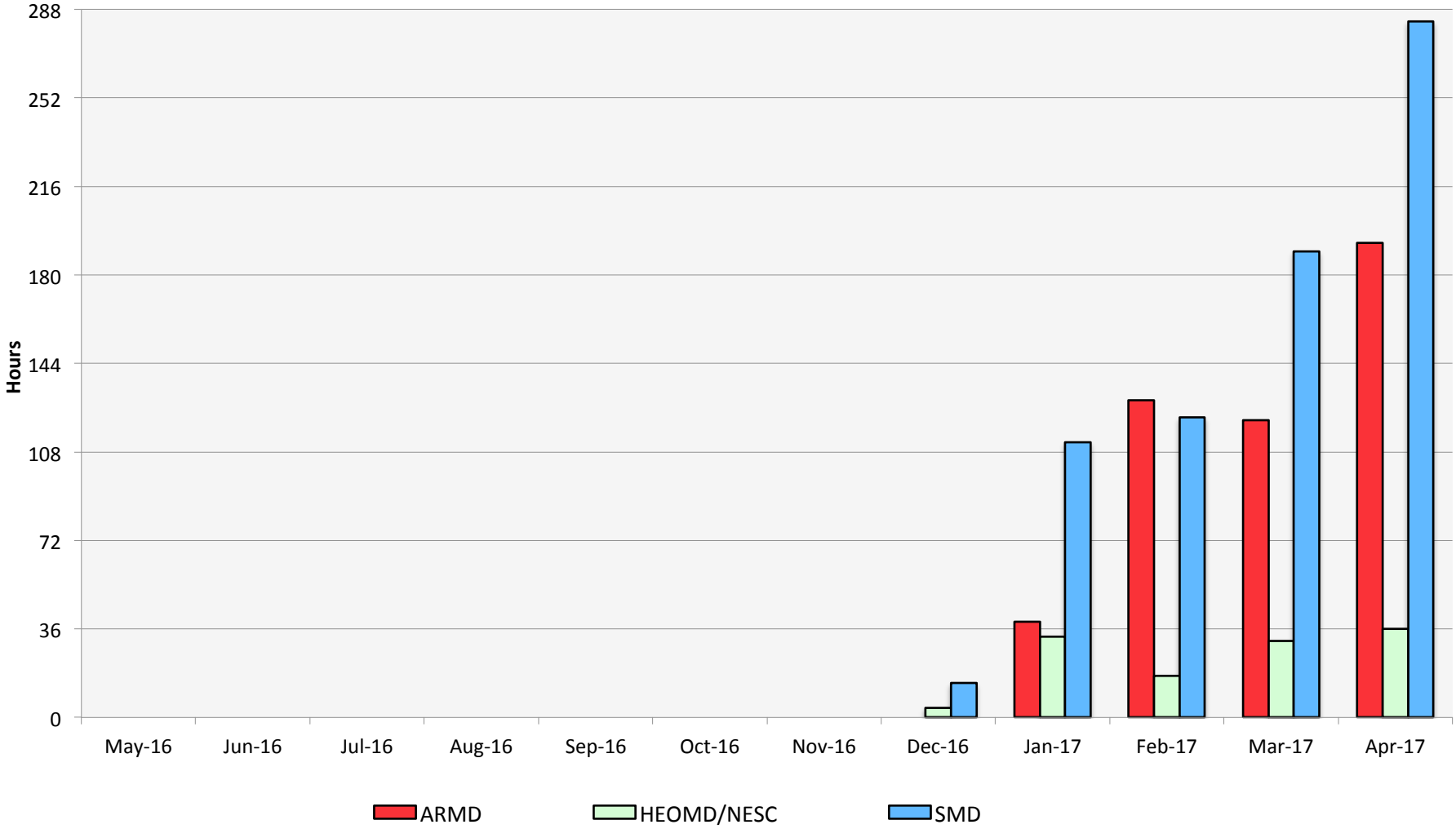
Electra:
Monthly Utilization by Size and Mission



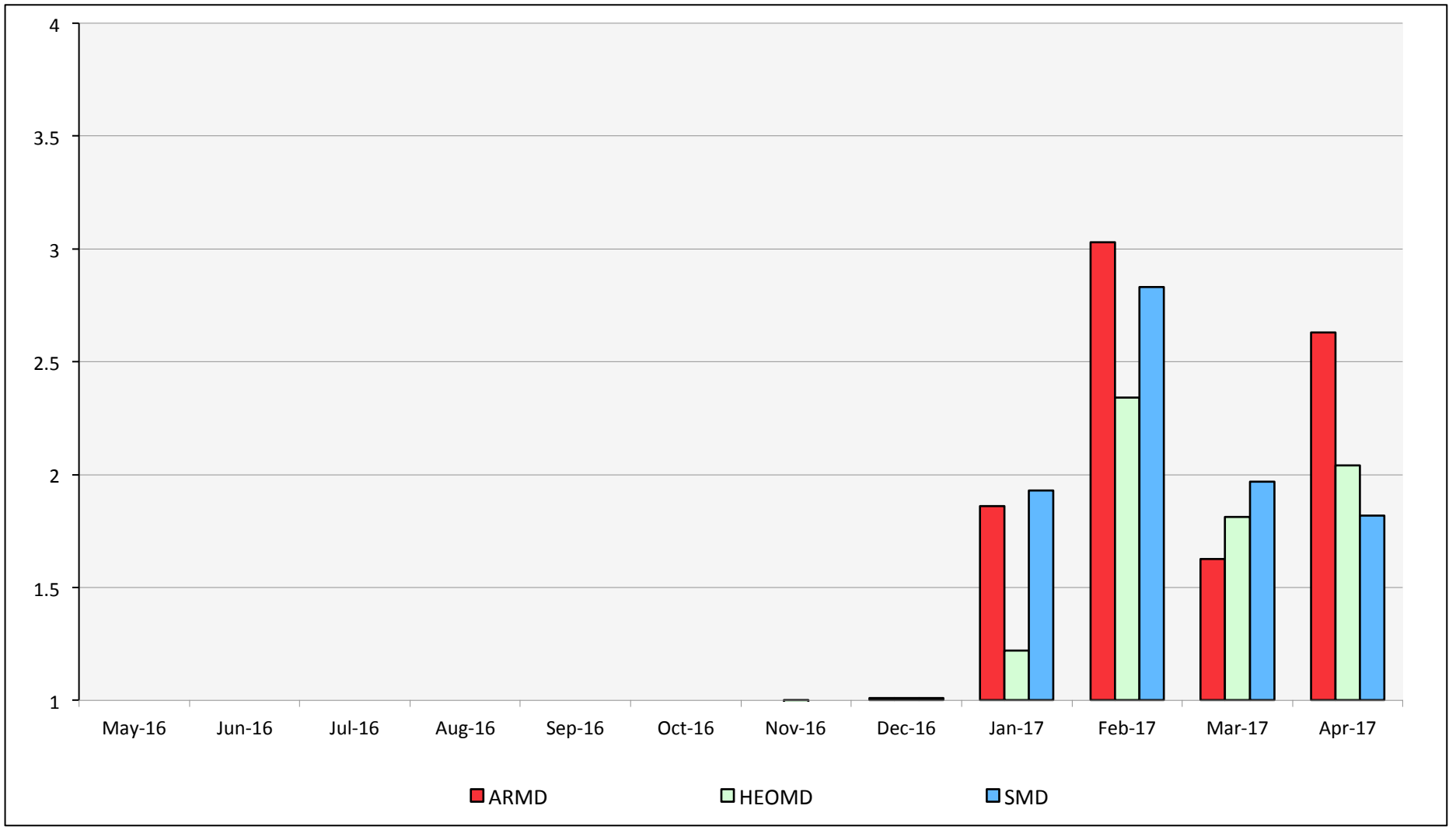
Electra:
Monthly Utilization by Size and Length



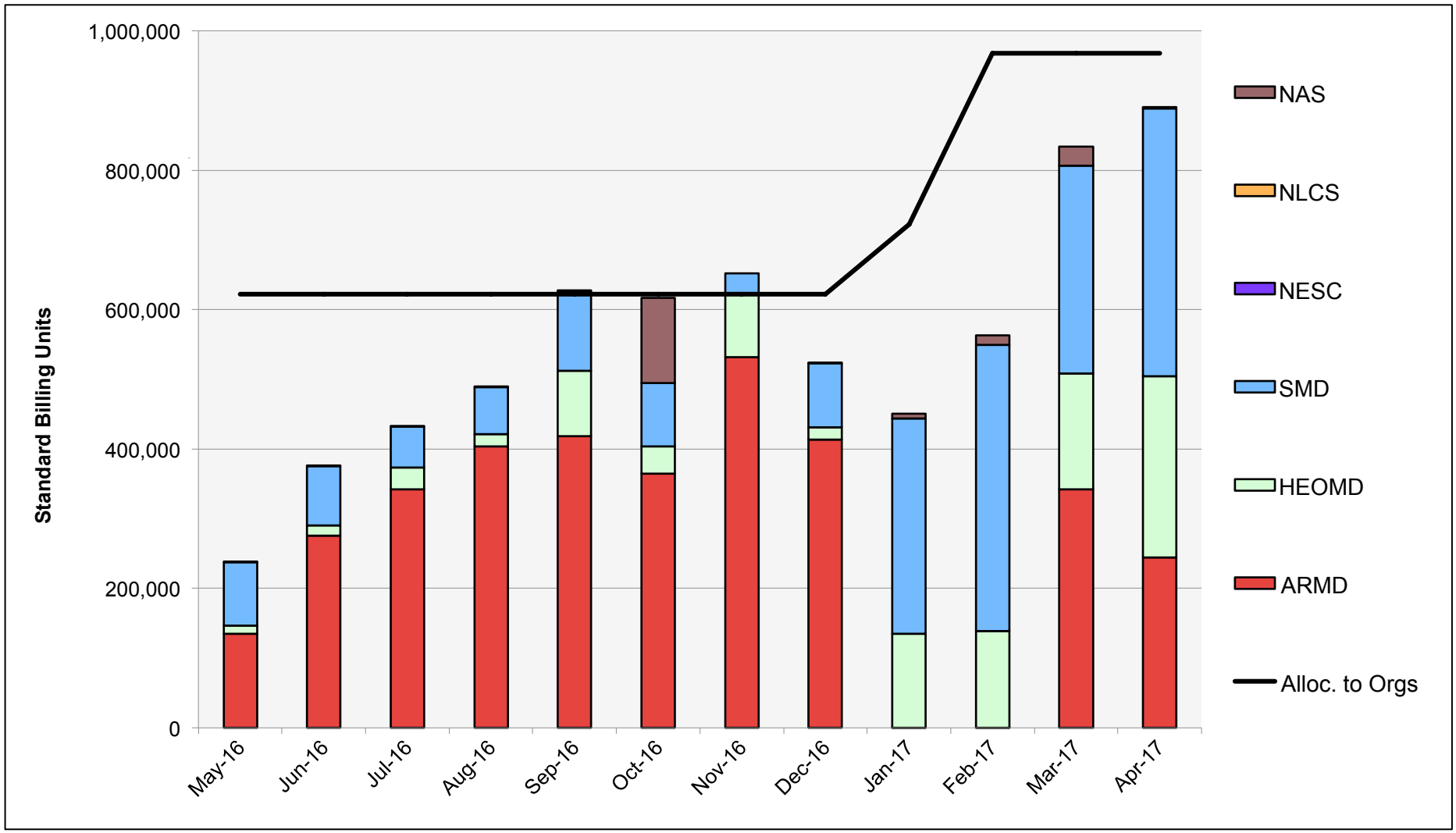
Electra:
Average Time to Clear All Jobs



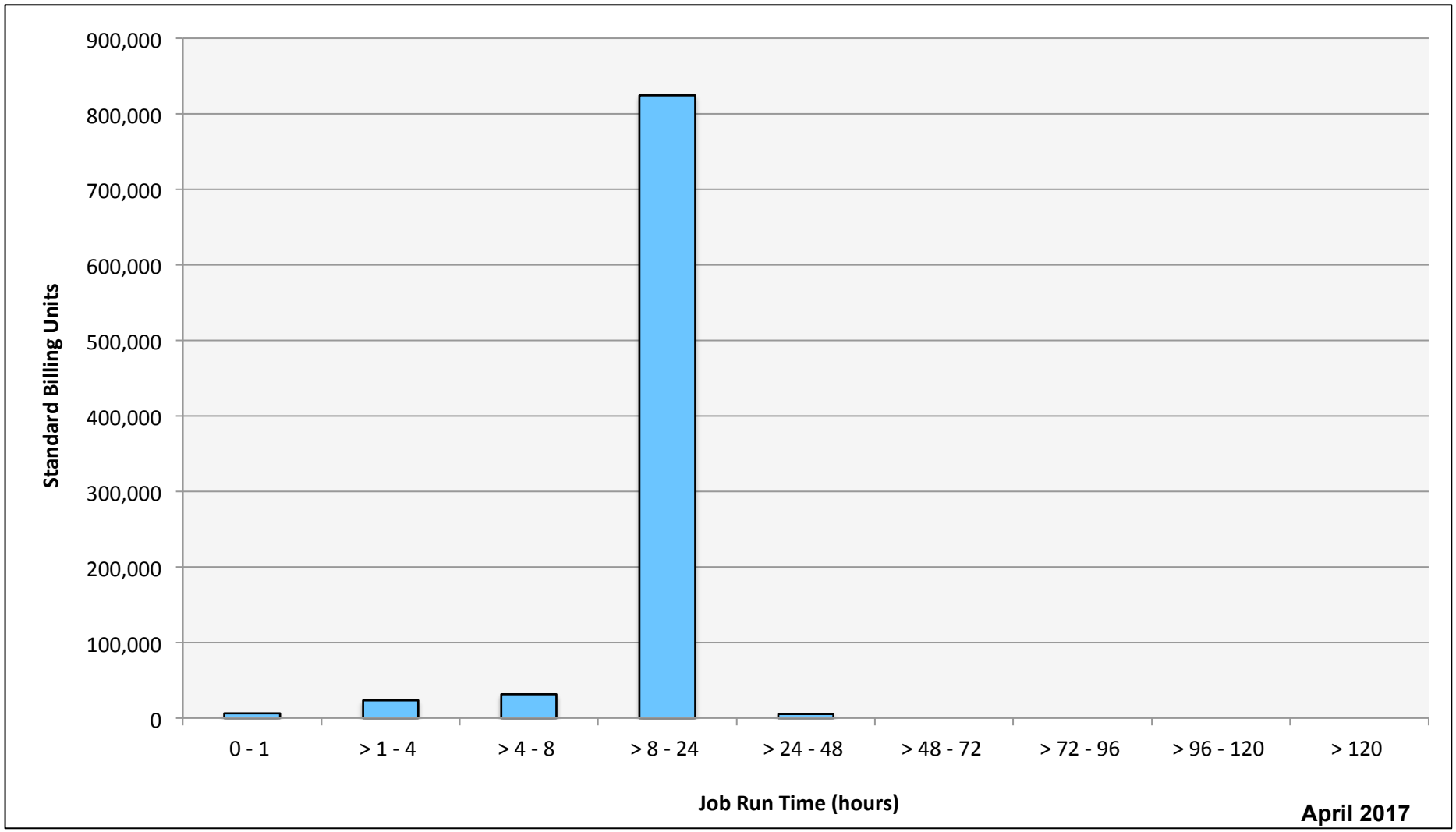
Electra:
Average Expansion Factor



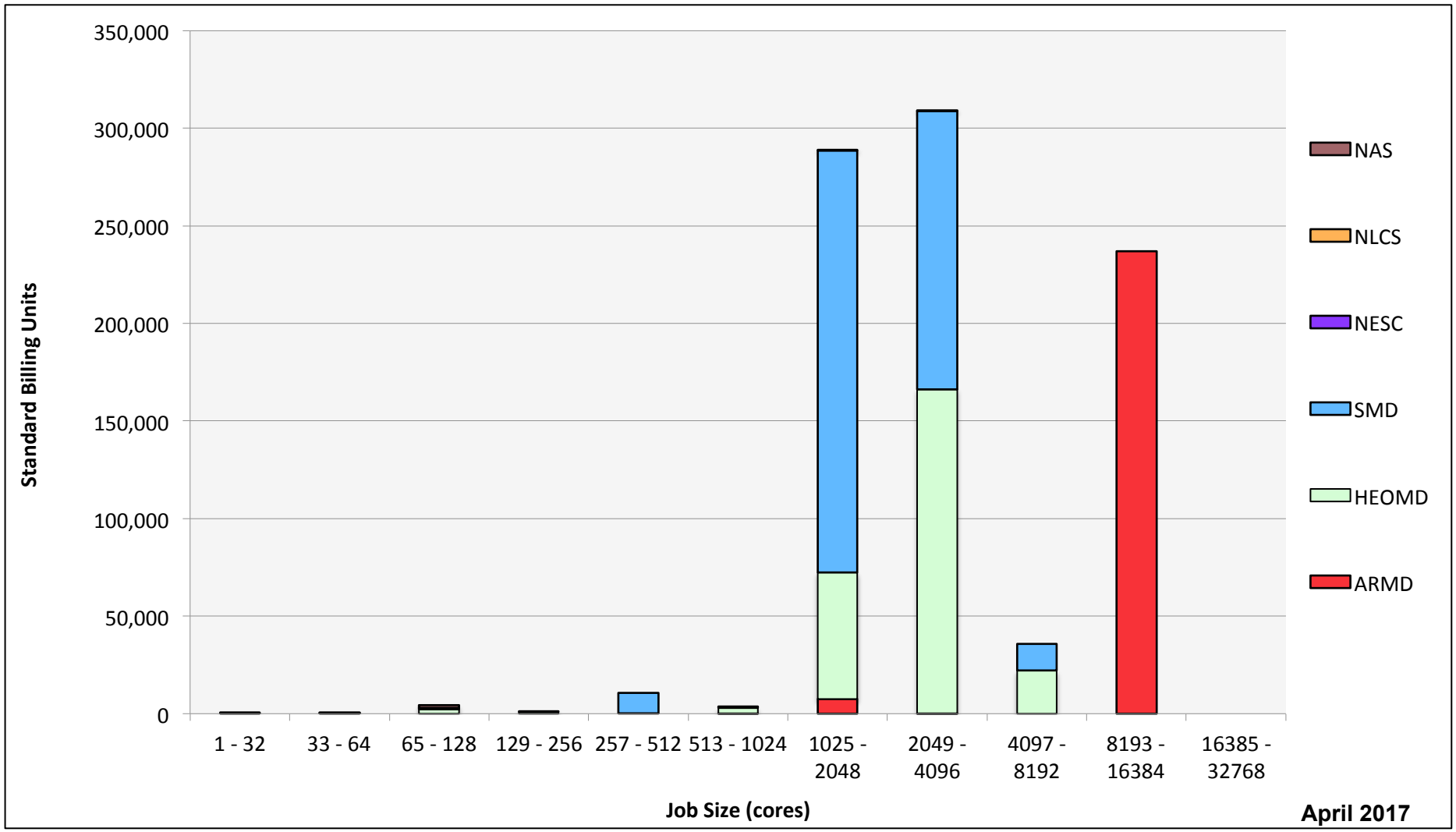
Merope:
SBUs Reported, Normalized to 30-Day Month



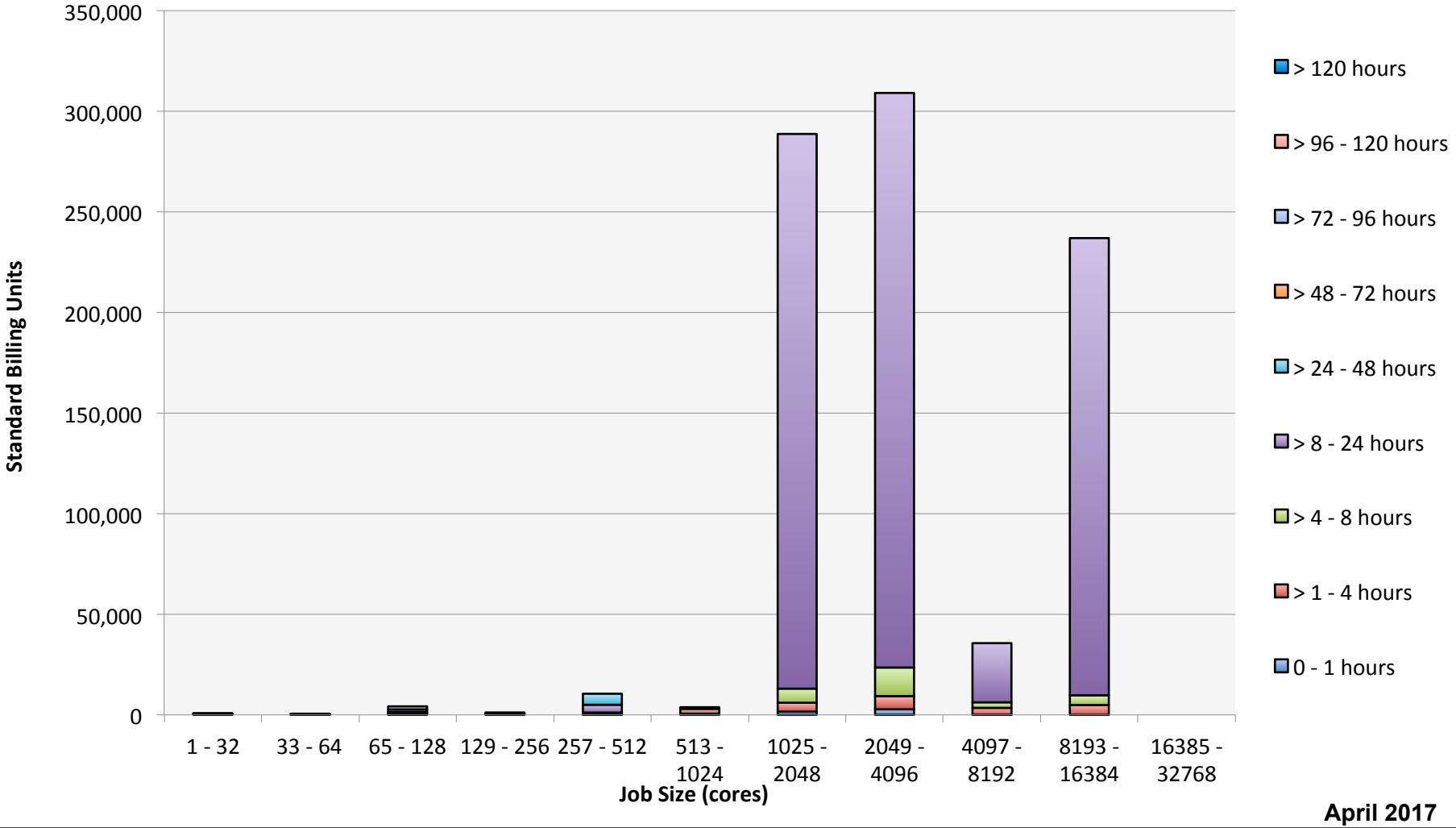
Merope:
Monthly Utilization by Job Length



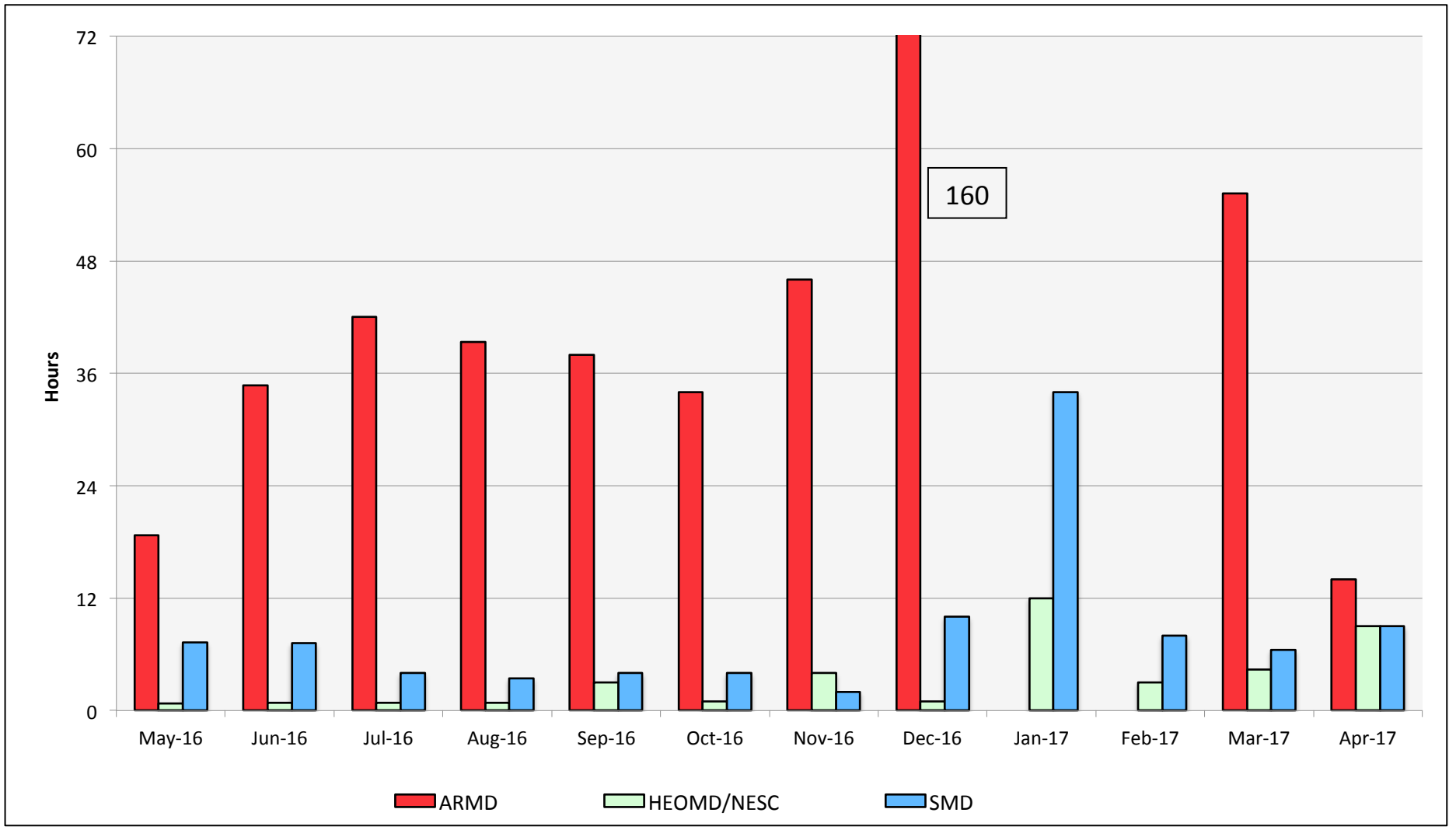
Merope:
Monthly Utilization by Size and Mission



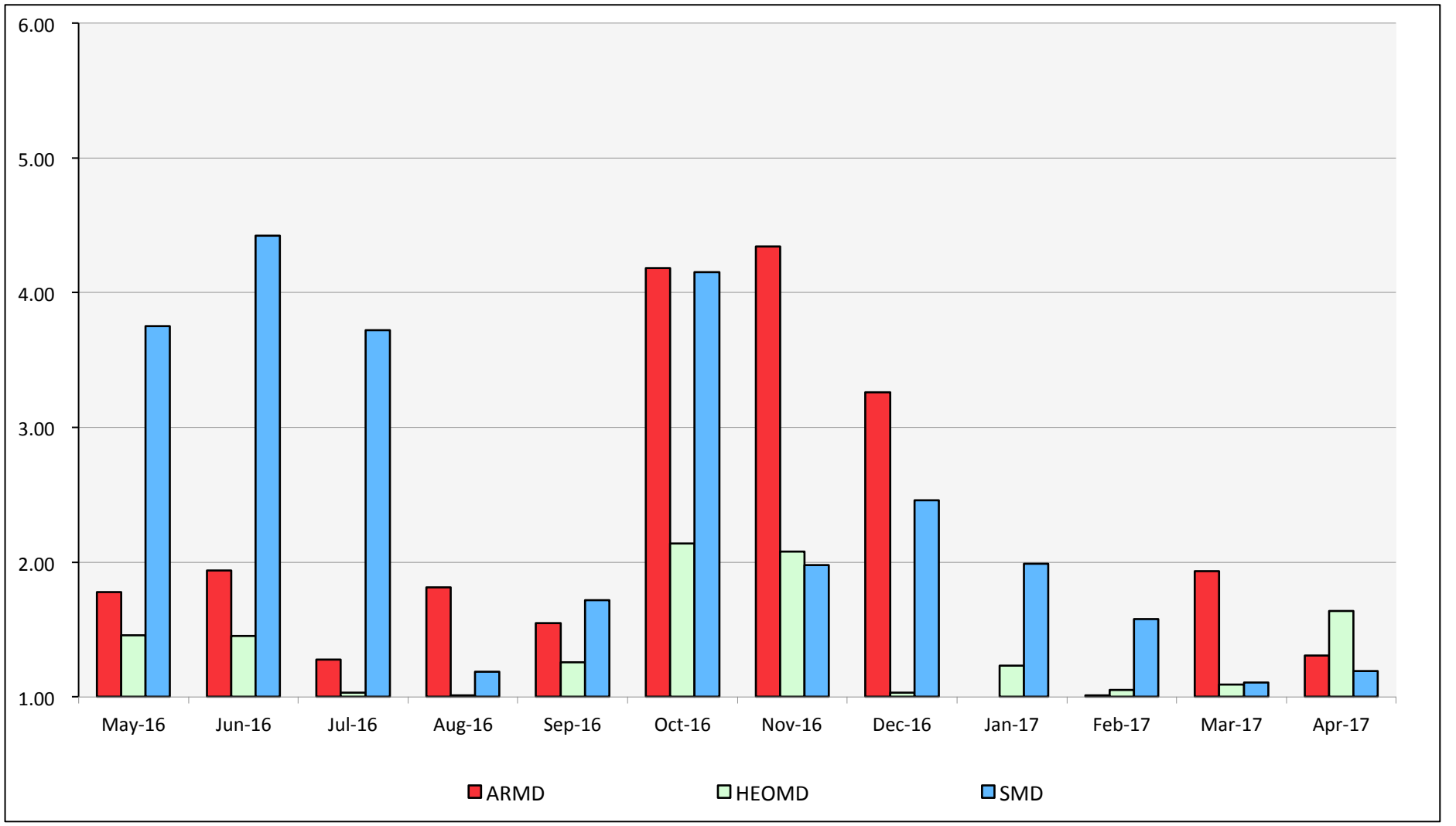
Merope:
Monthly Utilization by Size and Length



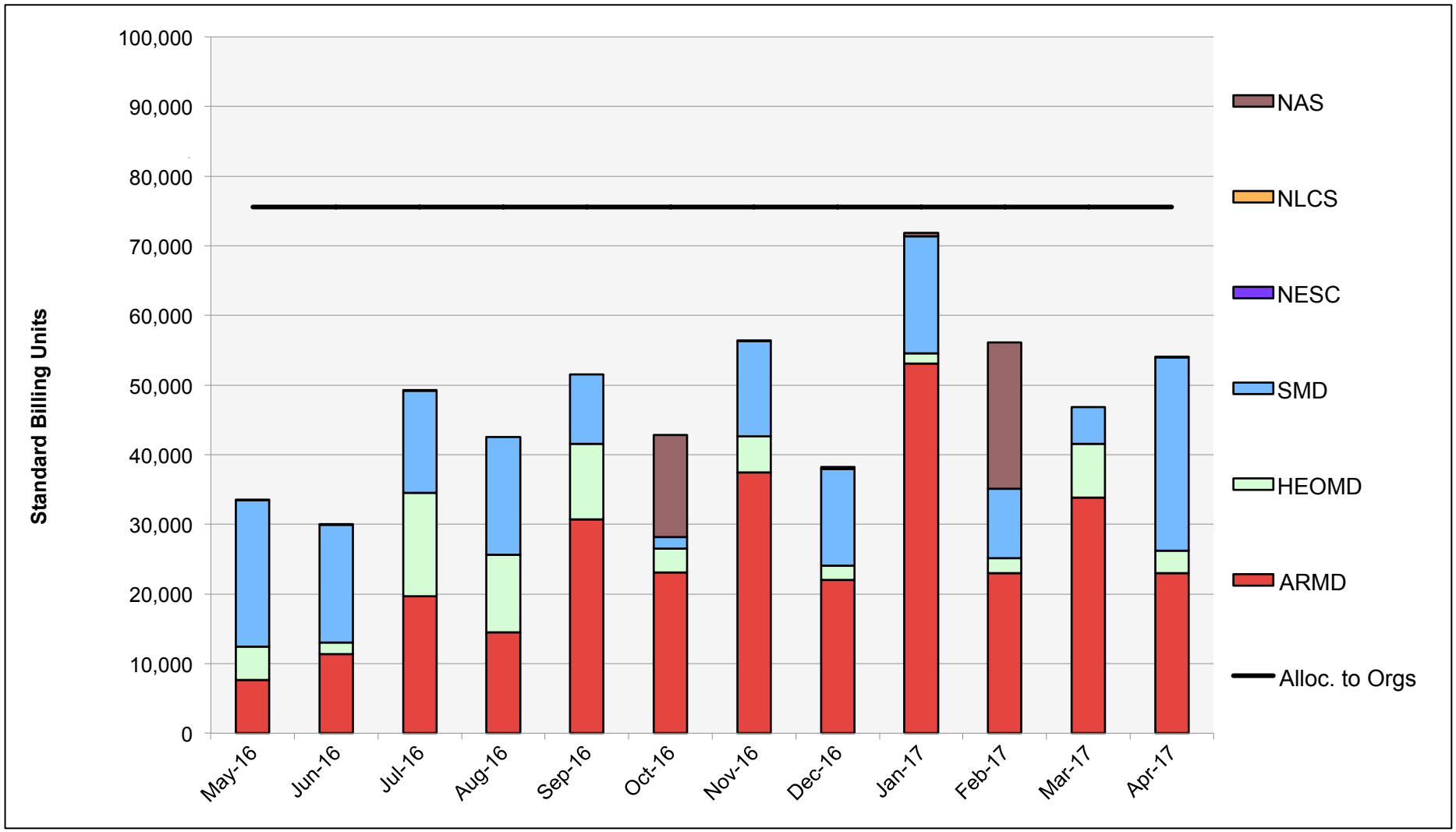
Merope:
Average Time to Clear All Jobs



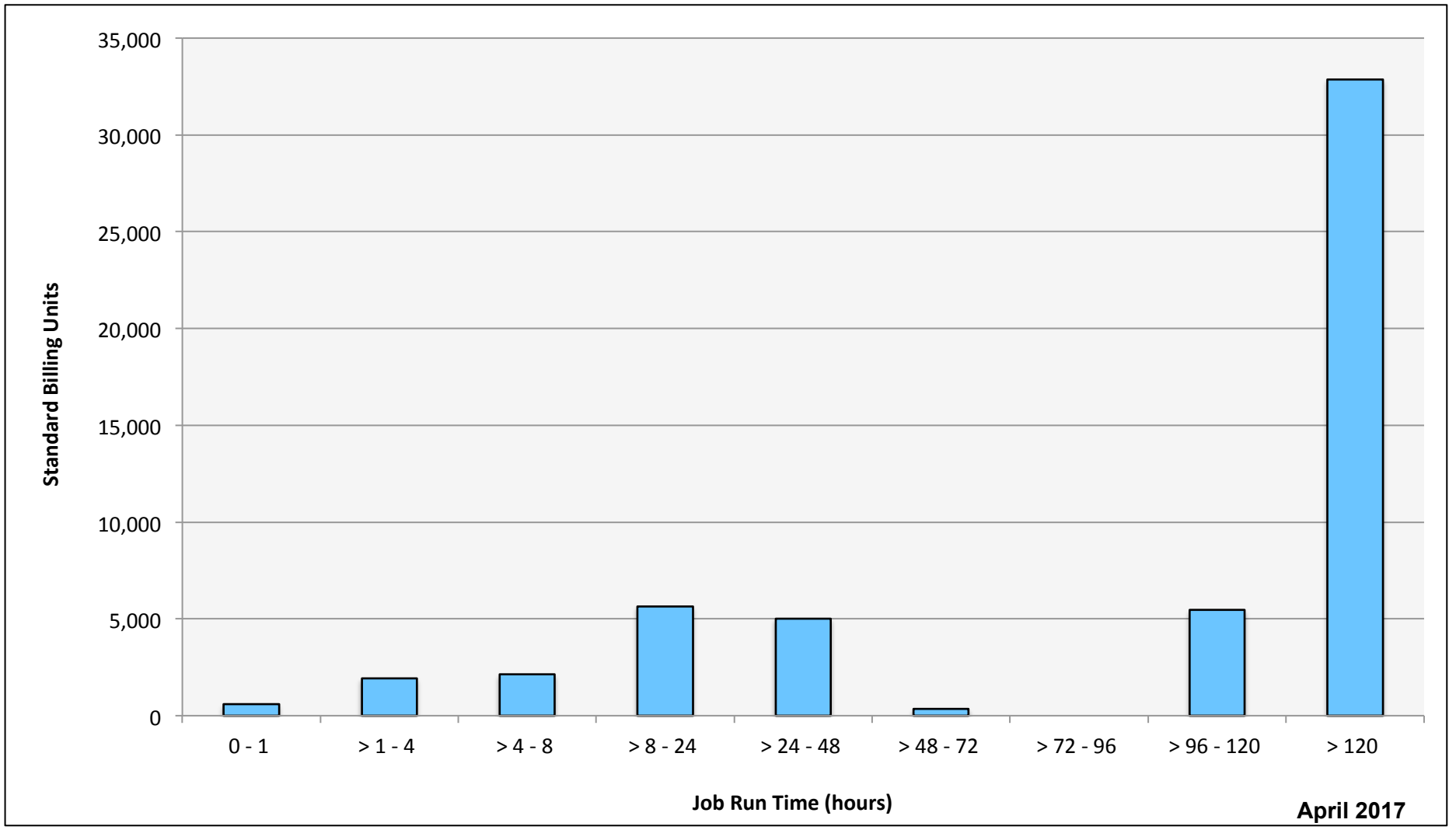
Merope:
Average Expansion Factor



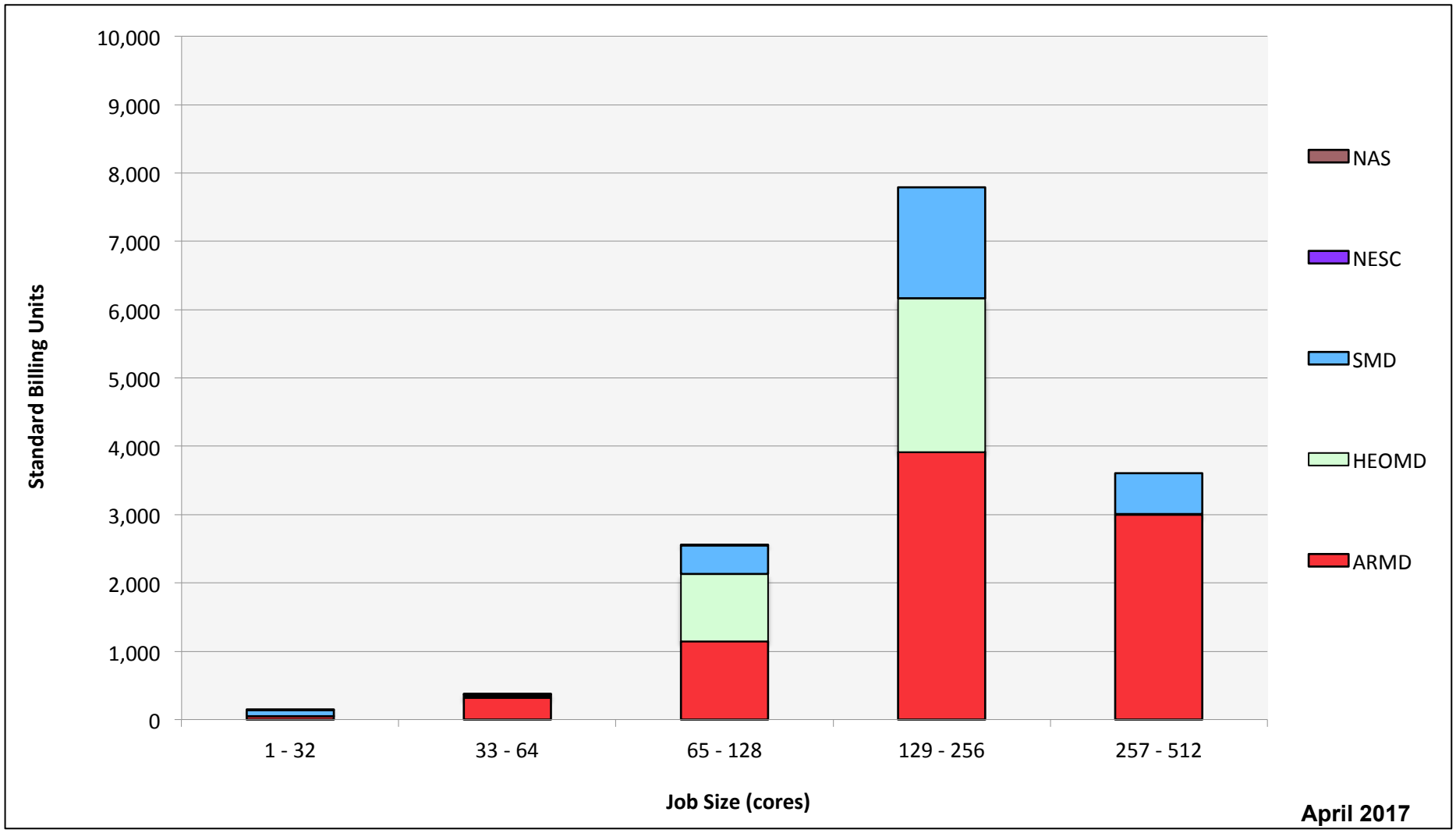
Endeavour:
SBUs Reported, Normalized to 30-Day Month



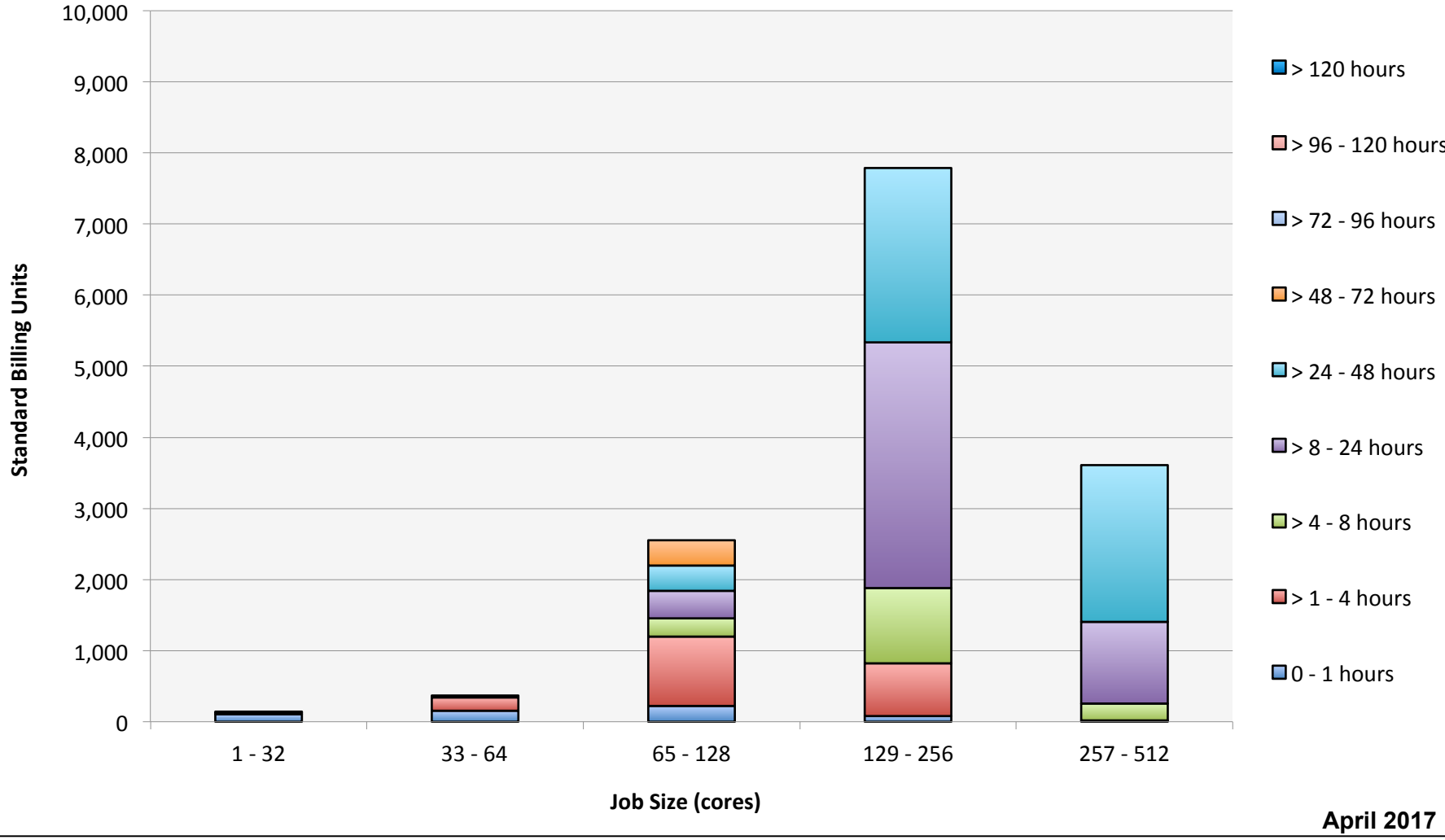
Endeavour:
Monthly Utilization by Job Length



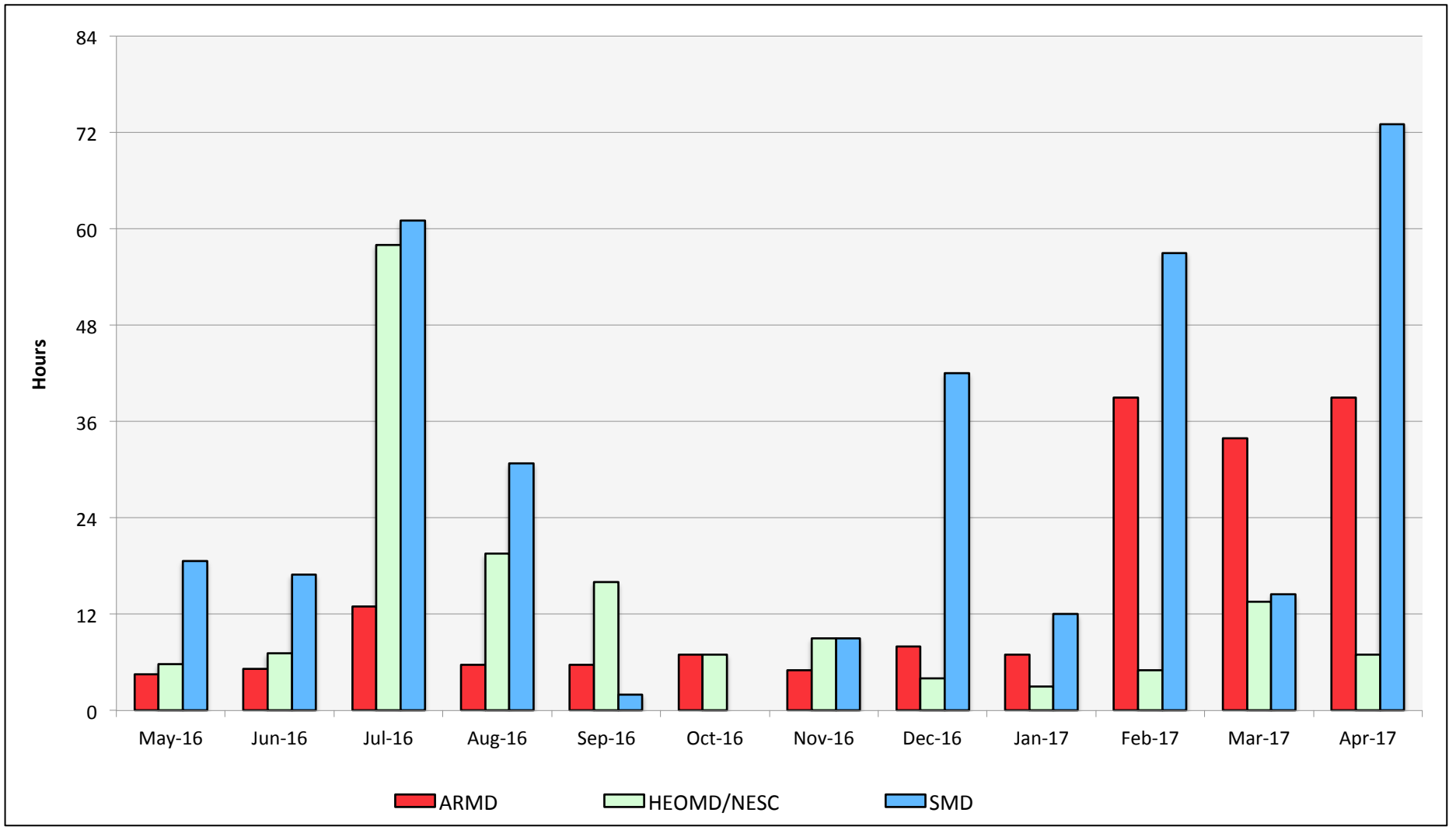
Endeavour:
Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length



Endeavour:
Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor